

Effect of Impurities with Internal Structure on Multiband Superconductors – Possible Enhancement of Transition Temperature –

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We study inelastic (dynamical) impurity scattering effects in two-band superconductors with the same (s_{++} wave) or different (s_{\pm} wave) sign order parameters. We focus on the enhancement of the superconducting transition temperature T_c by magnetic interband scattering with the interchange of crystal-field singlet ground and multiplet excited states. Either the s_{++} -wave or s_{\pm} -wave state is favored by the impurity-mediated pairing, which depends on the magnetic and nonmagnetic scattering strengths derived from the hybridization of the impurity states with the conduction bands. The details are examined for the singlet-triplet configuration that is suggestive of Pr impurities in the skutterudite superconductor $\text{LaOs}_4\text{Sb}_{12}$.

KEYWORDS: multiband superconductivity, s_{++} -wave superconductivity, s_{\pm} -wave superconductivity, heavy fermion, skutterudite, impurity, crystal field

1. Introduction

The study of impurity effects on multiband superconductivity is stimulated by the discovery of high-temperature (high T_c) superconductors with FeAs layers,^{1–8)} while it has been performed for another high- T_c superconductor, MgB_2 .^{9–11)} One of the interesting points for the impurity problem is their anisotropic band property. In particular, much attention is paid to the s_{\pm} -wave pairing state characterized by sign reversal of order parameters with full gaps.^{12–16)} For a depairing effect caused by impurity scattering, the s_{\pm} -wave state behaves like d -wave pairing rather than the conventional s -wave state.¹⁷⁾ Multiband properties are also reported in the heavy-fermion superconductor $\text{PrOs}_4\text{Sb}_{12}$ whose higher T_c than $\text{LaOs}_4\text{Sb}_{12}$ implies a crucial role of the Pr f -electron states.^{18,19)} Interband scattering due to impurities may be important in the multiband, the roles of which remain to be elucidated.

Recently, Senga and Kontani have studied the effects of intraband and interband nonmagnetic impurity scatterings in the s_{\pm} -wave state using a simple two-band BCS model.^{20,21)} They found that T_c is not markedly suppressed when the intraband and interband scattering strengths are not equal and are sufficiently strong. We also applied a similar model in a magnetic impurity case and solved a single-impurity problem.²²⁾ For the interband scattering in the s_{\pm} -wave state, the roles of magnetic impurities are equivalent to those of nonmagnetic impurities for the intraband scattering.¹⁷⁾ Very recently, it has been reported that T_c is not markedly suppressed so much by the interband magnetic scattering.²³⁾ These results imply a possibility of T_c enhancement due to magnetic impurities having an internal structure. Such enhancement was argued by Fulde *et al.* for nonmagnetic impurities in single-band superconductors.²⁴⁾ An attractive interaction stems from inelastic nonmagnetic scattering by impurities, which is analogous to the electron-phonon origin of BCS superconductors. T_c can

be enhanced by doping such impurities with appropriate crystal-field level splitting, while it is suppressed by magnetic impurities.²⁴⁾ This idea has recently been applied to a skutterudite superconductor $\text{La}_{1-x}\text{Pr}_x\text{Os}_4\text{Sb}_{12}$ to account for the T_c enhancement by Pr substitution for La in $\text{LaOs}_4\text{Sb}_{12}$.²⁵⁾ Since only a single band is considered there, one always finds that magnetic impurities cause T_c suppression. However, this conventional understanding has to be reexamined for multiband superconductors. In the case of s_{\pm} -wave superconductivity, magnetic impurities for intraband scattering behave like nonmagnetic impurities for interband scattering, and vice versa. Accordingly, we can expect T_c to be enhanced by the inelastic (dynamical) magnetic scattering.

In this paper, we extend the theory of Fulde *et al.*²⁴⁾ and show a case of magnetic impurities in the s_{\pm} -wave state in §2. Considering spin-dependent interband scattering, we examine a self-energy in the Born approximation to derive a gap equation for two bands. The increase in T_c is associated with the sign change of the superconducting order parameter via the inelastic impurity scattering. It is demonstrated for the s_{\pm} -wave state whose T_c is enhanced by the magnetic interband scattering due to the singlet-singlet configuration. In §3, we also show some typical examples of the corresponding interband scattering. There are various octupolar (combination of spin and orbital) scattering types that increase T_c accompanied by an interchange between two crystal-field singlet states. The same argument is applied to the singlet-multiplet configuration that can be realized for such f -electron impurities as rare-earth or actinide ions embedded in cubic or uniaxial anisotropic (tetragonal or hexagonal) crystals. For the singlet-doublet, we discuss the s_{\pm} -wave and s_{++} -wave combination via intraband scattering. The s_{++} -wave pairing is characterized by the same sign order parameters of the two bands. We show a possible crystal-field splitting for T_c enhancement, however, T_c is suppressed by the competition between mag-

netic and nonmagnetic scattering effects. For the singlet-triplet, we find a case in which the s_{++} wave is favorable for the T_c enhancement by magnetic interband scattering. Which is chosen, the s_{\pm} wave or the s_{++} wave, by the impurity-mediated pairing depends on (1) the scattering type (dipole, quadrupole, octupole, etc.) and (2) the hybridization between the impurity atomic orbitals and conduction bands. The details are described for an impurity with the singlet-triplet configuration. Its application to Pr impurity effects in the $\text{LaOs}_4\text{Sb}_{12}$ superconductor is discussed in §4. Conclusions are given in §5.

2. Formulation for T_c Enhancement

In this section, we present a formulation for T_c enhancement by inelastic impurity scattering in multiband superconductors. First, we briefly review a work by Fulde *et al.* for single-band superconductors.²⁴⁾ Then, we extend it to a two-band system as a simple case of multiband and give an example to understand multiband effects on T_c .

2.1 Inelastic impurity scattering and T_c enhancement in single-band superconductors

Let us begin with the model Hamiltonian $\mathcal{H} = \mathcal{H}_C + \mathcal{H}_I + \mathcal{H}'$ that consists of conduction electron \mathcal{H}_C , impurity \mathcal{H}_I , and impurity scattering \mathcal{H}' terms. The first term is written as

$$\mathcal{H}_C = \sum_{\sigma} \int d\mathbf{r} \psi_{\sigma}^{\dagger}(\mathbf{r}) \epsilon(-i\nabla) \psi_{\sigma}(\mathbf{r}) - \Delta \int d\mathbf{r} [\psi_{\uparrow}^{\dagger}(\mathbf{r}) \psi_{\downarrow}^{\dagger}(\mathbf{r}) + \psi_{\downarrow}(\mathbf{r}) \psi_{\uparrow}(\mathbf{r})]. \quad (1)$$

Here, $\psi_{\sigma}(\mathbf{r})$ is a field operator of the conduction electron of the $\sigma (= \uparrow, \downarrow)$ spin whose kinetic energy is expressed by the operator $\epsilon(i\nabla) = -\nabla^2/2m_e - E_F$ measured from the Fermi energy E_F , where m_e represents the electron mass and the Planck constant \hbar is taken as unity. Δ is the s -wave superconducting order parameter that we assume to be a real value. The Hamiltonian \mathcal{H}_I for the impurity states is given by

$$\mathcal{H}_I = \sum_{\mathbf{R}_{\gamma}} \sum_m \delta_m a_{\gamma m}^{\dagger} a_{\gamma m}. \quad (2)$$

Here, \mathbf{R}_{γ} represents the position of the γ th impurity. $a_{\gamma m}^{\dagger}$ and $a_{\gamma m}$ are the pseudo-fermion creation and annihilation operators, respectively, for the m th impurity energy level δ_m at the γ th impurity site.²⁶⁾ The interaction Hamiltonian at the impurities is defined by

$$\mathcal{H}' = \sum_{\mathbf{R}_{\gamma}} \sum_{mn} \sum_{\sigma} \int d\mathbf{r} a_{\gamma m}^{\dagger} a_{\gamma n} \delta(\mathbf{r} - \mathbf{R}_{\gamma}) M_{mn} \psi_{\sigma}^{\dagger}(\mathbf{r}) \psi_{\sigma}(\mathbf{r}). \quad (3)$$

We consider here only nonmagnetic impurity scattering since magnetic impurity scattering cannot enhance T_c in a single-band case.²⁴⁾ M_{mn} is a matrix element that describes the scattering of conduction electrons accompanied by an interchange among the m th and n th energy levels.

We introduce the following 4×4 matrix form of the

thermal Green's function:

$$\hat{G}(\tau, \mathbf{r}, \mathbf{r}') = -\langle T \Psi(\mathbf{r}, \tau) \Psi^{\dagger}(\mathbf{r}', 0) \rangle, \quad (4)$$

where $\Psi(\mathbf{r})$ and $\Psi^{\dagger}(\mathbf{r})$ are four-dimensional vectors defined as

$$\Psi(\mathbf{r}) = \begin{pmatrix} \psi_{\uparrow}(\mathbf{r}) \\ \psi_{\downarrow}(\mathbf{r}) \\ \psi_{\uparrow}^{\dagger}(\mathbf{r}) \\ \psi_{\downarrow}^{\dagger}(\mathbf{r}) \end{pmatrix}, \quad \Psi^{\dagger}(\mathbf{r}) = \begin{pmatrix} \psi_{\uparrow}^{\dagger}(\mathbf{r}) & \psi_{\downarrow}^{\dagger}(\mathbf{r}) & \psi_{\uparrow}(\mathbf{r}) & \psi_{\downarrow}(\mathbf{r}) \end{pmatrix}, \quad (5)$$

with their Heisenberg representations

$$\Psi(\mathbf{r}, \tau) = e^{\mathcal{H}\tau} \Psi(\mathbf{r}) e^{-\mathcal{H}\tau}, \quad \Psi^{\dagger}(\mathbf{r}, \tau) = e^{\mathcal{H}\tau} \Psi^{\dagger}(\mathbf{r}) e^{-\mathcal{H}\tau}. \quad (6)$$

In the absence of impurity scattering, the unperturbed Green's function is Fourier-transformed to

$$\hat{G}_0(i\omega_l, \mathbf{k}) = -\frac{i\omega_l + \epsilon_{\mathbf{k}} \hat{\rho}_3 + \Delta \hat{\rho}_2 \hat{\sigma}_2}{\omega_l^2 + \epsilon_{\mathbf{k}}^2 + \Delta^2}, \quad (7)$$

where $\hat{\sigma}_{\alpha}$ and $\hat{\rho}_{\alpha}$ (α is denoted by 1, 2, and 3 instead of x , y , and z , respectively, hereafter) are the Pauli matrices for the spin space and particle-hole space, respectively. Similarly, the matrix for impurity scattering is given by

$$\hat{U}_{mn} = M_{mn} \hat{\rho}_3. \quad (8)$$

Following Fulde *et al.*,²⁴⁾ we study the T_c enhancement on the basis of the second Born approximation. For the scattering matrix \hat{U}_{mn} in eq. (8), Fig. 1 shows the self-energy given by

$$\hat{\Sigma}(i\omega_l) = -n_{\text{imp}} T^2 \sum_{mn} \sum_{\omega_1 \omega_2} \frac{1}{i\omega_1 - \delta_m} \frac{1}{i\omega_2 - \delta_n} \times \frac{1}{\Omega} \sum_{\mathbf{k}} \hat{U}_{mn} \hat{G}_0(i\omega_l + i\omega_1 - i\omega_2, \mathbf{k}) \hat{U}_{nm}. \quad (9)$$

Here, n_{imp} represents the impurity density. $1/(i\omega_1 - \delta_m)$ is an unperturbed Green's function for the m th impurity energy level. ω_1 and ω_2 are Matsubara frequencies for fermions. Ω represents the system volume. The Boltzmann constant k_B is taken as unity. The important point is that Δ in eq. (7) changes its sign with the $\hat{U}_{mn} \hat{G}_0 \hat{U}_{nm}$ transformation. This is a key to the T_c enhancement due to the inelastic impurity scattering, by analogy with the optical phonon case leading to an attractive interaction for pairing.²⁴⁾ On the other hand, for the elastic impurity scattering, the pairing interaction is cancelled out by a depairing effect.

In the presence of the impurities, the linearized gap equation is given by

$$\Delta \log \frac{T_c}{T_{c0}} = \pi T_c \sum_l \frac{\Delta}{|\omega_l|} \left[\Sigma_{\Delta}(i\omega_l) - i \frac{\Sigma_{\omega}(i\omega_l)}{\omega_l} \right], \quad (10)$$

where T_c (T_{c0}) is the transition temperature in the presence (absence) of impurities. Σ_{Δ} and Σ_{ω} are self-energies corresponding to the order parameter and Matsubara frequency components, respectively.²⁴⁾ In Green's function, the renormalized frequency $\tilde{\omega}_l$ and the order parameter

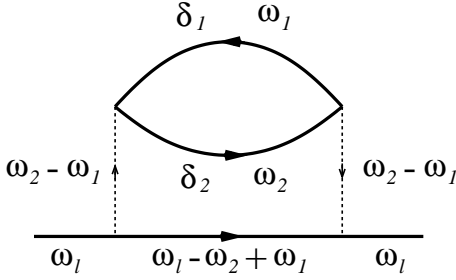


Fig. 1. Feynman diagram of self-energy in the second Born approximation.

$\tilde{\Delta}_l$ are given by

$$\tilde{\omega}_l = \omega_l + i\Sigma_\omega(i\omega_l), \quad \tilde{\Delta}_l = \Delta[1 + \Sigma_\Delta(i\omega_l)]. \quad (11)$$

The self-energy in Fig. 1 leads to different signs of Σ_Δ in eq. (10) between time-reversal invariant scattering and non-time-reversal invariant scattering.²⁴⁾ The former (nonmagnetic scattering in a single band) contributes to T_c enhancement. In a simple case of two energy levels ($\delta_2 > \delta_1$), after the lengthy calculation of the self-energy, we obtain each term on the right-hand side of eq. (10) as

$$\begin{aligned} \pi T_c \sum_l \frac{1}{|\omega_l|} \Sigma_\Delta(i\omega_l) &= -\frac{\pi}{8T_c \tau_{12}} f_\Delta(x), \\ f_\Delta(x) &= -\frac{\tanh x}{x} + A(x) - \frac{1}{2}B(x), \\ \pi T_c \sum_l \frac{i}{|\omega_l|} \frac{\Sigma_\omega(i\omega_l)}{\omega_l} &= -\frac{\pi}{8T_c \tau_{12}} f_\omega(x), \\ f_\omega(x) &= -1 + \tanh^2 x - \frac{1}{2}B(x), \\ \frac{1}{\tau_{12}} &= 2\pi n_{\text{imp}} N_0 |M_{12}|^2, \end{aligned} \quad (12)$$

with

$$x = \frac{\delta_2 - \delta_1}{2T_c} > 0, \quad A(x) = S_1(x) \tanh x, \quad B(x) = S_2(x) \tanh x. \quad (13)$$

$$\begin{aligned} S_1(x) &= \frac{4x}{\pi^4} \text{Re} \sum_{n=0}^{\infty} \frac{\psi\left(1 + n - i\frac{x}{\pi}\right) - \psi\left(\frac{1}{2}\right)}{\left(n + \frac{1}{2}\right) \left(n + \frac{1}{2} - i\frac{x}{\pi}\right)^2}, \\ S_2(x) &= \frac{8}{\pi^3} \text{Im} \sum_{n=0}^{\infty} \frac{\psi\left(1 + n - i\frac{x}{\pi}\right) - \psi\left(\frac{1}{2}\right)}{\left(n + \frac{1}{2} - i\frac{x}{\pi}\right)^2}. \end{aligned}$$

Here, τ_{12} represents the lifetime due to the impurity scattering. N_0 is the density of states at the Fermi energy. $\psi(x)$ is the digamma function. As a consequence, eq. (10) leads to a gap equation for the nonmagnetic scattering (τ_{12} is denoted by τ_{12}^0),

$$\frac{8T_c}{\pi} \tau_{12}^0 \log \frac{T_c}{T_{c0}} = -f_\Delta(x) + f_\omega(x) \equiv f_0(x) > 0, \quad (14)$$

and to that for the magnetic scattering (τ_{12} is denoted by τ_{12}^s),

$$\frac{8T_c}{\pi} \tau_{12}^s \log \frac{T_c}{T_{c0}} = f_\Delta(x) + f_\omega(x) \equiv -f_s(x) < 0. \quad (15)$$

These equations show that for any finite crystal-field splitting, T_c is enhanced by nonmagnetic impurities in single-band s -wave superconductors, while it is suppressed by magnetic impurities.²⁴⁾ For the nonmagnetic scattering in eq. (14), we note that T_c keeps T_{c0} for $x = 0$ (elastic scattering) that gives $f_0(0) = 0$ [$f_\Delta(0) = f_\omega(0) = -1$], while $|f_\Delta(x)| > |f_\omega(x)|$ [$f_\Delta(x) < 0, f_\omega(x) < 0$] for $x > 0$ leads to $T_c > T_{c0}$. Once the two levels are split, the exchange scattering process gives rise to an attractive interaction for pairing, by analogy with the optical phonon effects in superconductivity.²⁴⁾

We would like to mention a linear combination of eqs. (14) and (15), $[f_0(x)/\tau_{12}^0 + f_s(x)/\tau_{12}^s]$, which is derived from the singlet-multiplet configuration since both magnetic and nonmagnetic scatterings coexist. In this case, the weight of $f_\Delta(x)$ becomes smaller in the combined equation, so that x has to be sufficiently large to satisfy the condition $|f_\Delta(x)| > |f_\omega(x)|$ for T_c enhancement. The details will be examined for the singlet-doublet configuration in §3.2.

2.2 Extension to multiband superconductors

2.2.1 Bulk property

Before extending the above single-band case to a two-band one, we briefly review the earlier works by Shul *et al.*²⁷⁾ and Kondo²⁸⁾ for multiband superconductivity. The unique property of the multiband is described by the following model Hamiltonian:

$$\begin{aligned} \mathcal{H}_{\text{bulk}} &= \sum_{\mu=\pm} \sum_{\sigma=\uparrow,\downarrow} \sum_{\mathbf{k}} \epsilon_{\mathbf{k}\mu\sigma} c_{\mathbf{k}\mu\sigma}^\dagger c_{\mathbf{k}\mu\sigma} \\ &+ \sum_{\mu,\mu'=\pm} \sum_{\mathbf{k}\mathbf{k}'} V_{\mu\mu'} c_{\mathbf{k}\mu\uparrow}^\dagger c_{-\mathbf{k}\mu\downarrow}^\dagger c_{-\mathbf{k}'\mu'\downarrow} c_{\mathbf{k}'\mu'\uparrow}. \end{aligned} \quad (16)$$

Here, the first term represents the kinetic energy for the $\mu (= \pm)$ conduction band and $c_{\mathbf{k}\mu\sigma}^\dagger$ ($c_{\mathbf{k}\mu\sigma}$) is the creation (annihilation) operator. The second term represents the interaction between electrons with coupling constants $V_{\mu\mu'}$: $\mu = \mu'$ for the intraband and $\mu \neq \mu'$ for the interband. T_c is determined by the following form of the linearized gap equation:

$$\begin{aligned} \begin{pmatrix} -V_{++}N_{0+} & -V_{+-}N_{0-} \\ -V_{-+}N_{0+} & -V_{--}N_{0-} \end{pmatrix} \begin{pmatrix} \Delta_+ \\ \Delta_- \end{pmatrix} \\ = \frac{1}{\log[(2e^\gamma \omega_c)/(\pi T_c)]} \begin{pmatrix} \Delta_+ \\ \Delta_- \end{pmatrix}. \end{aligned} \quad (17)$$

Here, Δ_\pm and $N_{0\pm}$ are the order parameters and density of states at the Fermi energy for the $\mu = \pm$ band, respectively. $\gamma (\simeq 0.577)$ is Euler's constant and we have assumed the same cut-off energy $\omega_c (\gg T_c)$ for the two bands. T_c corresponds to a positive eigenvalue of the 2×2 matrix on the left-hand side of eq. (17). The multiband superconductivity is characterized by whether the interband interaction is attractive or repulsive. To see this point clearly, let us consider a simple case of two identical bands, where $V_{++} = V_{--} < 0$, $V_{+-} = V_{-+}$, and

$N_{0+} = N_{0-} = N_0$. The solution of eq. (17) is obtained as

$$\begin{aligned} T_{cA} &= \frac{2e^{\gamma\omega_c}}{\pi} \exp \left[-\frac{1}{(|V_{++}| - V_{+-})N_0} \right], \\ T_{cB} &= \frac{2e^{\gamma\omega_c}}{\pi} \exp \left[-\frac{1}{(|V_{++}| + V_{+-})N_0} \right]. \end{aligned} \quad (18)$$

Here, T_{cA} and T_{cB} are the transition temperatures for

$$\Delta_A = \frac{\Delta_+ + \Delta_-}{2}, \quad \Delta_B = \frac{\Delta_+ - \Delta_-}{2}, \quad (19)$$

respectively. When $V_{+-} < 0$, $T_{cA} > T_{cB}$ ($T_{cB} = 0$ if $|V_{+-}| > |V_{++}|$). This means that the higher T_c is due to the attractive interband interaction for the order parameters with the same sign ($\Delta_+\Delta_- > 0$). Conversely, when $V_{+-} > 0$, the higher T_c is obtained for their opposite signs ($\Delta_+\Delta_- < 0$). The former and latter are called the s_{++} -wave and s_{\pm} -wave states, respectively.

2.2.2 Impurity effect

Although electron-phonon and Coulomb interactions were taken into account as possible origins of the interband interaction before,^{27,28)} we here propose inelastic (dynamical) impurity scattering as another origin that can give rise to T_c enhancement in multiband superconductors even if it is due to magnetic impurities. For this purpose, we extend the work by Fulde *et al.* to a two-band case.

Then, we reexamine the gap equation in eq. (10) for a two-band s -wave superconducting state with order parameters, Δ_μ for the μ band. In the absence of impurities, the superconducting transition temperatures are expressed as $T_{c0\pm}$ for the $\mu = \pm$ bands, respectively. Here, the interband interaction is not taken into account for simplicity ($V_{+-} = 0$). Considering both magnetic and nonmagnetic scattering processes, we obtain the following linearized gap equation in the two-band case:

$$\begin{aligned} \frac{8T_c}{\pi} \begin{pmatrix} \Delta_+ \log \frac{T_c}{T_{c0+}} \\ \Delta_- \log \frac{T_c}{T_{c0-}} \end{pmatrix} \\ = \sum_{X=0,s} \frac{1}{\tau_{12}^X} \left[f_\Delta(x) \hat{\lambda}_\Delta^X + f_\omega(x) \hat{\lambda}_\omega^X \right] \begin{pmatrix} \Delta_+ \\ \Delta_- \end{pmatrix}, \end{aligned} \quad (20)$$

where T_c is the transition temperature in the presence of impurities. The energy difference x between the impurity singlet ground and multiplet excited states is scaled by $2T_c$ [see eq. (13)]. The matrices $\hat{\lambda}_\Delta^X$ and $\hat{\lambda}_\omega^X$ express the impurity intraband and interband scattering contributions to the self-energies, $\Sigma_\Delta(i\omega)$ and $\Sigma_\omega(i\omega)$, respectively:

$$\hat{\lambda}_\xi^X = \begin{pmatrix} \lambda_{\xi,++}^X & \lambda_{\xi,+ -}^X \\ \lambda_{\xi,- +}^X & \lambda_{\xi,--}^X \end{pmatrix} \quad (\xi = \Delta, \omega). \quad (21)$$

In the following study, it is convenient to use the order parameters given in eq. (19), where Δ_A and Δ_B are order parameters for the s_{++} -wave and s_{\pm} -wave states,

respectively. By the unitary transformation

$$\hat{\lambda}_\xi^X = U^{-1} \hat{\lambda}_\xi^X U, \quad U = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}, \quad (22)$$

the linearized gap equation is rewritten as

$$\begin{aligned} \left[\frac{1}{2} \log \left(\frac{T_{c0+}}{T_{c0-}} \right) \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} + \hat{\Lambda}(x) \right] \begin{pmatrix} \Delta_A \\ \Delta_B \end{pmatrix} \\ = \frac{8T_c}{\pi} \log \left(\frac{T_c}{\sqrt{T_{c0+}T_{c0-}}} \right) \begin{pmatrix} \Delta_A \\ \Delta_B \end{pmatrix}, \end{aligned} \quad (23)$$

$$\hat{\Lambda}(x) = \sum_{X=0,s} \frac{1}{\tau_{12}^X} \sum_{\xi=\Delta,\omega} f_\xi(x) \hat{\lambda}_\xi^X.$$

We can see that T_c , which is the superconducting transition temperature in the presence of impurities, plays a role as an eigenvalue of the matrix on the left-hand side in eq. (23). The largest eigenvalue corresponds to the highest T_c . When $T_{c0+} = T_{c0-}$ for simplicity, only $\hat{\Lambda}(x)$ is left on the left-hand side, and a positive eigenvalue of $\hat{\Lambda}$ leads to T_c enhancement.

Next, we consider a case of two identical bands with interband interaction ($V_{+-} \neq 0$). In this case, the T_c values are different for the s_{++} -wave and s_{\pm} -wave states, as given by eq. (18). In the absence of impurities, we introduce transition temperatures T_{c0A} and T_{c0B} for the s_{++} and s_{\pm} -wave states, respectively. For T_c in the presence of impurities, the gap equation is expressed as

$$\begin{aligned} \left[\frac{1}{2} \log \left(\frac{T_{c0A}}{T_{c0B}} \right) \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} + \hat{\Lambda}(x) \right] \begin{pmatrix} \Delta_A \\ \Delta_B \end{pmatrix} \\ = \frac{8T_c}{\pi} \log \left(\frac{T_c}{\sqrt{T_{c0A}T_{c0B}}} \right) \begin{pmatrix} \Delta_A \\ \Delta_B \end{pmatrix}. \end{aligned} \quad (24)$$

Here, the contribution of the impurities is expressed by $\hat{\Lambda}(x)$ and it modifies the transition temperatures in the bulk.

In the following part of this paper, we consider only two identical bands without the interband scattering ($V_{+-} = 0$) to capture the essence of the T_c enhancement caused by the inelastic scattering impurities, where $T_{c0A} = T_{c0B} = T_{c0}$. We note that it is easy to extend the formulation to $T_{c0A} \neq T_{c0B}$ cases.

2.3 Example of magnetic interband scattering for T_c enhancement in s_{\pm} -wave state

As mentioned above, T_c is enhanced by inelastic non-magnetic impurity scattering in single-band s -wave superconductors. In this subsection, we show that magnetic interband scattering can also cause T_c enhancement in multiband cases. For this purpose, we focus on the roles of spin-dependent scattering in the s_{\pm} -wave state, which is suggested as one of possible superconducting states realized in Fe pnictide superconductors.^{12,13)} As we will see, the interband scattering is important for T_c enhancement, which is unique to the multiband and is never seen in the single-band case. In fact, neither intraband nor elastic impurity scattering can be neglected in real systems. These effects cause T_c suppression. Whether T_c is enhanced or not depends on how to balance the pairing and depairing effects caused by impurities.

Here, we extend the formulation given in §2.1 straightforwardly. The conduction electron part for the μ band is given by

$$\begin{aligned} \mathcal{H}_\mu &= \sum_\sigma \int d\mathbf{r} \psi_{\mu\sigma}^\dagger(\mathbf{r}) \epsilon(-i\nabla) \psi_{\mu\sigma}(\mathbf{r}) \\ &\quad - \Delta_\mu \int d\mathbf{r} \left[\psi_{\mu\uparrow}^\dagger(\mathbf{r}) \psi_{\mu\downarrow}^\dagger(\mathbf{r}) + \psi_{\mu\downarrow}(\mathbf{r}) \psi_{\mu\uparrow}(\mathbf{r}) \right] \\ &\quad (\mu = +, -). \end{aligned} \quad (25)$$

Here, $\psi_{\mu\sigma}(\mathbf{r})$ is a field operator of the conduction electron for the μ band. Δ_μ is the μ band superconducting order parameter for the s_\pm -wave superconductivity, where Δ_μ takes a real value. For spin-dependent intraband and interband scatterings at the impurities, the interaction Hamiltonian is defined by

$$\begin{aligned} \mathcal{H}' &= \sum_{\mathbf{R}_\gamma} \sum_{mn} \sum_{\mu\nu} \sum_{\sigma\sigma'} \int d\mathbf{r} a_{\gamma m}^\dagger a_{\gamma n} \delta(\mathbf{r} - \mathbf{R}_\gamma) \\ &\quad \times \mathbf{M}_{mn,\mu\nu} \cdot \hat{\boldsymbol{\sigma}}_{\sigma\sigma'} \psi_{\mu\sigma}^\dagger(\mathbf{r}) \psi_{\nu\sigma'}(\mathbf{r}), \end{aligned} \quad (26)$$

where $\hat{\boldsymbol{\sigma}}$ is the Pauli matrix with the three components $\hat{\sigma}_\alpha$ ($\alpha = 1, 2, 3$). As the corresponding spin exchange, $\mathbf{M}_{mn,\mu\nu}$ is the scattering matrix element that depends on the band components as well.

We introduce the following 4×4 matrix form of the thermal Green's function for the μ band:

$$\hat{G}_\mu(\tau, \mathbf{r}, \mathbf{r}') = -\langle T \Psi_\mu(\mathbf{r}, \tau) \Psi_\mu^\dagger(\mathbf{r}', 0) \rangle, \quad (27)$$

where $\Psi_\mu(\mathbf{r})$ and $\Psi_\mu^\dagger(\mathbf{r})$ are defined for each band as

$$\begin{aligned} \Psi_\mu(\mathbf{r}) &= \begin{pmatrix} \psi_{\mu\uparrow}(\mathbf{r}) \\ \psi_{\mu\downarrow}(\mathbf{r}) \\ \psi_{\mu\uparrow}^\dagger(\mathbf{r}) \\ \psi_{\mu\downarrow}^\dagger(\mathbf{r}) \end{pmatrix}, \\ \Psi_\mu^\dagger(\mathbf{r}) &= \begin{pmatrix} \psi_{\mu\uparrow}^\dagger(\mathbf{r}) & \psi_{\mu\downarrow}^\dagger(\mathbf{r}) & \psi_{\mu\uparrow}(\mathbf{r}) & \psi_{\mu\downarrow}(\mathbf{r}) \end{pmatrix} \end{aligned} \quad (28)$$

Their Heisenberg representations $\Psi_\mu(\mathbf{r}, \tau)$ and $\Psi_\mu^\dagger(\mathbf{r}, \tau)$ are given in the same manner as eq. (6). After introducing the unperturbed Green's function

$$\hat{G}_\mu(i\omega_l, \mathbf{k}) = -\frac{i\omega_l + \epsilon_{\mathbf{k}} \hat{\rho}_3 + \Delta_\mu \hat{\rho}_2 \hat{\sigma}_2}{\omega_l^2 + \epsilon_{\mathbf{k}}^2 + \Delta_\mu^2}, \quad (29)$$

as in eq. (7), and combining the two-band forms, we use the following 8×8 matrix form of Green's function:

$$\hat{G}_0(i\omega_l, \mathbf{k}) = \begin{pmatrix} \hat{G}_+(i\omega_l, \mathbf{k}) & 0 \\ 0 & \hat{G}_-(i\omega_l, \mathbf{k}) \end{pmatrix}. \quad (30)$$

In particular, for the s_\pm -wave state ($\Delta_+ = -\Delta_- = \Delta$), it is rewritten as

$$\hat{G}_0(i\omega_l, \mathbf{k}) = -\frac{i\omega_l + \epsilon_{\mathbf{k}} \hat{\rho}_3 + \Delta \hat{\tau}_3 \hat{\rho}_2 \hat{\sigma}_2}{\omega_l^2 + \epsilon_{\mathbf{k}}^2 + \Delta^2}, \quad (31)$$

where $\hat{\tau}_\alpha$ ($\alpha = 1, 2, 3$) is the Pauli matrix for the band space. Similarly, the matrix for impurity scattering is given by, for instance,

$$\begin{aligned} \hat{U} &= \sum_{mn} \sum_{\alpha=x,y,z} \hat{U}_{mn}^\alpha, \\ \hat{U}_{mn}^x &= M_{mn}^x \hat{\tau}_1 \hat{\rho}_3 \hat{\sigma}_1, \quad \hat{U}_{mn}^y = M_{mn}^y \hat{\tau}_1 \hat{\sigma}_2, \end{aligned}$$

$$\hat{U}_{mn}^z = M_{mn}^z \hat{\tau}_1 \hat{\rho}_3 \hat{\sigma}_3. \quad (32)$$

Here, $\hat{\tau}_1$ represents the interband scattering. For the scattering matrix \hat{U} in eq. (32), the self-energy in Fig. 1 is given by

$$\begin{aligned} \hat{\Sigma}(i\omega_l) &= -n_{\text{imp}} T^2 \sum_{mn} \sum_{\omega_1 \omega_2} \frac{1}{i\omega_1 - \delta_m} \frac{1}{i\omega_2 - \delta_n} \\ &\quad \times \frac{1}{\Omega} \sum_{\mathbf{k}} \sum_{\alpha} \hat{U}_{mn}^\alpha \hat{G}_0(i\omega_l + i\omega_1 - i\omega_2, \mathbf{k}) \hat{U}_{nm}^\alpha. \end{aligned} \quad (33)$$

As in the single-band case, Δ in eq. (31) changes its sign by the $\hat{U}_{mn}^\alpha \hat{G}_0 \hat{U}_{nm}^\alpha$ transformation. This is a key to the T_c enhancement by inelastic scattering also in the multiband case.

We apply the above argument to the spin-dependent interband scattering case such as eq. (32) that enhances the T_c of the s_\pm -wave superconductivity. In the calculation of the self-energy, the scattering matrix \hat{U}_{mn}^α satisfies

$$\begin{aligned} \hat{U}_{mn}^\alpha (\Delta \hat{\tau}_3 \hat{\rho}_2 \hat{\sigma}_2) \hat{U}_{nm}^\alpha &= -|M_{mn}^\alpha|^2 (\Delta \hat{\tau}_3 \hat{\rho}_2 \hat{\sigma}_2), \\ \hat{U}_{mn}^\alpha \hat{U}_{nm}^\alpha &= |M_{mn}^\alpha|^2, \end{aligned} \quad (34)$$

which leads to

$$\hat{\Lambda}_\Delta^s = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \hat{\Lambda}_\omega^s = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad (35)$$

$$\frac{1}{\tau_{12}^s} = 2\pi n_{\text{imp}} N_0 \sum_{\alpha} |M_{12}^\alpha|^2, \quad (36)$$

in eq. (24). Here, N_0 represents the density of normal electron states at the Fermi energy. We have assumed here a singlet-singlet configuration for the energy levels ($m, n = 1, 2$) of the impurity. Then, we obtain the following gap equation:

$$\alpha_s \begin{pmatrix} -f_s(x) & 0 \\ 0 & f_0(x) \end{pmatrix} \begin{pmatrix} \Delta_A \\ \Delta_B \end{pmatrix} = \frac{T_c}{T_{c0}} \log \frac{T_c}{T_{c0}} \begin{pmatrix} \Delta_A \\ \Delta_B \end{pmatrix}, \quad (37)$$

where $x = (\delta_2 - \delta_1)/(2T_c)$ and α_s represents the strength of the spin-dependent impurity scattering defined by

$$\alpha_s = \frac{\pi}{8T_{c0}\tau_{12}^s}. \quad (38)$$

In the gap equation, $f_0(x) = -f_\Delta(x) + f_\omega(x) > 0$ and $f_s(x) = -f_\Delta(x) - f_\omega(x) > 0$ [see eqs. (14) and (15)]. This means that T_c is enhanced for the s_\pm -wave state. We show the $(\delta_2 - \delta_1)$ dependence of T_c for various α_s values in Fig. 2. At $\delta_1 = \delta_2$, where the two impurity states are degenerate, there is no T_c enhancement. When $(\delta_2 - \delta_1)$ is increased, T_c increases accordingly and takes a maximum value. In fact, T_c depends on two factors competing with each other. One is the strength of the attractive interaction between electrons as derived in the BCS theory. The other is the energy region for the attractive interaction related to the cutoff. The former is intensified by a small $(\delta_2 - \delta_1)$, while the latter becomes large for a large $(\delta_2 - \delta_1)$. In Fig. 2, one can see the maximum at approximately $(\delta_2 - \delta_1) \simeq 10T_{c0}$. For $(\delta_2 - \delta_1) \rightarrow \infty$, there is no enhancement in T_c , since such a higher-lying energy level does not contribute to the attractive interaction.

Thus, the order of $(\delta_2 - \delta_1) \sim T_c$ is the most appro-

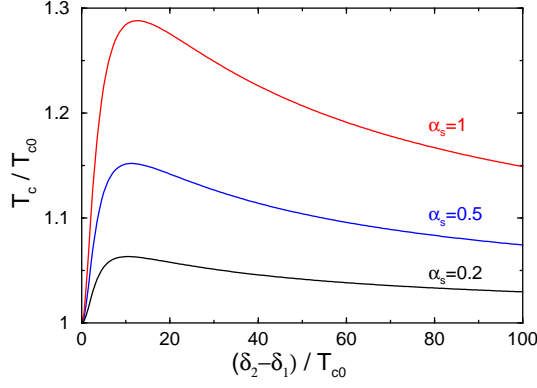


Fig. 2. (Color online) $(\delta_2 - \delta_1)$ dependence of T_c for various values of α_s .

appropriate for T_c enhancement by the interband scattering in the s_{\pm} -wave state. On the other hand, it must be pointed out that T_c suppression is caused by elastic scattering due to the impurity singlet ground state or by intraband scattering [for instance, $\hat{\tau}_1$ is replaced by unity in eq. (32)], which have been neglected here. The most important point is the internal structure of impurities that intensifies the interband magnetic scattering to overcome these pair-breaking effects.

3. Typical Impurity Interband Scattering for T_c Enhancement

In §2.3, we have discussed T_c enhancement due to the spin-dependent interband scattering in s_{\pm} -wave states as one of the examples, where the details of such impurity scattering have been put aside. In this section, we study typical impurity scattering for a singlet-multiplet configuration that can give rise to T_c enhancement in multiband superconductors. First, we show possible examples for the singlet-singlet and next apply the same argument to the singlet-multiplet case. In §3.2, we take account of not only the interband impurity scattering effect but also the intraband impurity scattering effect neglected in the previous section.

3.1 Singlet-singlet configuration

In addition to the $\hat{\tau}_1$ type in eq. (32) for the interband scattering, there is another type of magnetic scattering, $M_{mn}\hat{\tau}_2$, due to an orbital moment (spin-independent scattering). Since it satisfies

$$\hat{\tau}_2(\hat{\tau}_3\hat{\rho}_2\hat{\sigma}_2)\hat{\tau}_2 = -(\hat{\tau}_3\hat{\rho}_2\hat{\sigma}_2), \quad (39)$$

T_c can be enhanced by the impurity scattering for the s_{\pm} wave. Here, we consider realistic cases for $\hat{U}_{mn}^z = M_{mn}^z\hat{\tau}_1\hat{\rho}_3\hat{\sigma}_3$ and $\hat{U}_{mn} = M_{mn}\hat{\tau}_2$. In practice, we check the possible symmetry of M_{12} for the singlet-singlet configuration corresponding to each electron scattering type, assuming local orbital symmetries of band electrons at the impurity site. Although actual bands can include several orbital components, we represent each band by an orbital component that mainly contributes to the band construction.

First, let us begin with the spin-dependent case, $\hat{U}_{mn}^z = M_{mn}^z\hat{\tau}_1\hat{\rho}_3\hat{\sigma}_3$. Within the subspace, $\psi_b =$

$(\psi_{+\uparrow} \ \psi_{+\downarrow} \ \psi_{-\uparrow} \ \psi_{-\downarrow})^t$, where t denotes transposition, \hat{U}_{mn}^z is given as

$$\hat{U}_{mn}^z = M_{mn}^z\hat{\tau}_1\hat{\sigma}_3 = M_{mn}^z \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix}. \quad (40)$$

To identify the symmetry of electron scattering that depends on orbital components, we here assume the yz and xz orbital types for the $\mu = +$ and $\mu = -$ bands, respectively. The wave functions $\psi_{yz,\sigma}$ and $\psi_{xz,\sigma}$ at an impurity are connected to $j = 3/2$ angular momentum bases ψ_{j_z} (specifically, the $O_h \Gamma_8$ point-group bases) by the following unitary transformation as

$$\begin{pmatrix} \psi_{yz\uparrow} \\ \psi_{xz\uparrow} \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} i & i \\ 1 & -1 \end{pmatrix} \begin{pmatrix} \psi_{3/2} \\ \psi_{-1/2} \end{pmatrix},$$

$$\begin{pmatrix} \psi_{yz\downarrow} \\ \psi_{xz\downarrow} \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} -i & -i \\ -1 & 1 \end{pmatrix} \begin{pmatrix} \psi_{1/2} \\ \psi_{-3/2} \end{pmatrix}. \quad (41)$$

In this new basis set $\psi_{j=3/2} = (\psi_{3/2} \ \psi_{1/2} \ \psi_{-1/2} \ \psi_{-3/2})^t$, it is useful to classify the scattering types (dipole, quadrupole, and octupole). \hat{U}_{mn}^z in eq. (40) is transformed as

$$\hat{U}_{mn}^z \rightarrow M_{mn}^z \begin{pmatrix} 0 & 0 & i & 0 \\ 0 & 0 & 0 & -i \\ -i & 0 & 0 & 0 \\ 0 & i & 0 & 0 \end{pmatrix}_{j=3/2 \text{ space}}. \quad (42)$$

This matrix expression corresponds to the xyz type of tensor for $j = 3/2$. In the local scattering at the impurity, M_{mn}^z has the same symmetry as xyz . In the cubic point group, M_{mn}^z expresses $O_h \Gamma_2$ octupole coupling (Γ_3 for D_{4h} point group). This coupling is realized in the f^2 configuration (doubly occupied f -electron state). For instance, it connects the D_{4h} crystal-field ground state

$$|g\rangle = c_1(|4\rangle + |-4\rangle) + c_2|0\rangle \quad (2|c_1|^2 + |c_2|^2 = 1), \quad (43)$$

with the first excited state

$$|e\rangle = \frac{1}{\sqrt{2}}(|2\rangle + |-2\rangle), \quad (44)$$

in the inelastic impurity scattering \hat{U}_{mn}^z . Here, $|M\rangle$ ($M = -4 \sim 4$) is an eigenstate of J_z for the $J = 4$ angular momentum state in the f^2 configuration. Within the two crystal-field states, the scattering matrix is expressed by

$$\begin{pmatrix} M_{11}^z & M_{12}^z \\ M_{21}^z & M_{22}^z \end{pmatrix} = |M_{12}^z| \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}. \quad (45)$$

Next, we consider the spin-independent case, $\hat{U}_{mn} = M_{mn}\hat{\tau}_2$. In the subspace ψ_b , we obtain

$$\hat{U}_{mn} = M_{mn} \begin{pmatrix} 0 & 0 & -i & 0 \\ 0 & 0 & 0 & -i \\ i & 0 & 0 & 0 \\ 0 & i & 0 & 0 \end{pmatrix}. \quad (46)$$

Assuming the yz and xz types for the two bands in this case as well, \hat{U}_{mn} is transformed to the $j = 3/2$ angular

momentum basis expression as

$$\hat{U}_{mn} \rightarrow M_{mn} \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}_{j=3/2 \text{ space}}, \quad (47)$$

which expresses the combination of the z dipole and $z(2z^2 - 3x^2 - 3y^2)$ octupole types of $j = 3/2$ electron scattering. For the inelastic impurity scattering in this case, M_{mn} represents the dipole coupling between two low-lying singlet states, e.g., the ground state $|g\rangle$ in eq. (43) and the excited state,

$$|e\rangle = \frac{1}{\sqrt{2}}(|4\rangle - |-4\rangle), \quad (48)$$

given as

$$\begin{pmatrix} M_{11} & M_{12} \\ M_{21} & M_{22} \end{pmatrix} = |M_{12}| \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}. \quad (49)$$

Finally, we mention another pair of two-band types, $(2z^2 - x^2 - y^2)$ and $(x^2 - y^2)$. Applying the above argument, we find that the $\hat{\tau}_1\hat{\rho}_3\hat{\sigma}_3$ type of electron scattering is reduced to the $z(x^2 - y^2)$ octupole type, and the $\hat{\tau}_2$ type corresponds to the xyz octupole type expressed by eq. (42). In Appendix A, we give a different analysis for \hat{U}_{mn}^z .

3.2 Singlet-doublet configuration

Here, we devote ourselves to extending the present theory of T_c enhancement to typical examples of impurities with internal degrees of freedom. Orbital degrees of freedom of conduction electrons give rise to magnetic and nonmagnetic exchange scatterings, both of which are considered here in the singlet-multiplet configuration. Whether T_c is enhanced or suppressed depends on the ratio of their scattering strengths that determines the signs of the two-band superconducting order parameters: they are the same ($\Delta_+\Delta_- > 0$) or different ($\Delta_+\Delta_- < 0$). For the T_c enhancement, the crystal-field ground state must be a singlet (a nonmagnetic doublet is also allowed). As mentioned for the s_{\pm} -wave state ($\Delta_+\Delta_- < 0$) in §2.3, T_c suppression is caused by elastic scattering due to the singlet, which is neglected here as well. First, we discuss a case of singlet-doublet configuration regarded as an $S = 1$ local pseudo-spin. This $S = 1$ spin is not a spin triplet but a spin and orbitally coupled state, as often studied for f -electron systems. The latter can be realized as an impurity low-lying state in a uniaxial (D_{4h} or D_{6h}) crystal field. In the same framework, we tackle a more complicated case of singlet-triplet configuration discussed in the next subsection.

For spin and orbitally coupled impurity states, in general, local orbital exchange occurs as well as spin exchange during electron scattering by the impurity moment. In the case of an $S^I = 1$ pseudo-spin for an impurity, a spherical type of exchange interaction is expressed by coupling with, for instance, local $S^c = 3/2$ states, $\psi^c = (\psi_{3/2} \ \psi_{1/2} \ \psi_{-1/2} \ \psi_{-3/2})^t$, formed by conduction electrons. This local interaction Hamiltonian is

given by²⁹⁾

$$H_{\text{loc}} = \psi^c \left(J_S \mathbf{S}^I \cdot \mathbf{S}^c + J_Q \sum_{\eta=1}^5 Q_{\eta}^I Q_{\eta}^c \right) \psi^c + \frac{1}{3} \Delta_{\text{CF}} [3 (S_z^I)^2 - 2], \quad (50)$$

where a potential (elastic) scattering term is neglected. The first and second terms represent dipolar and quadrupolar exchanges with the coupling constants, J_S and J_Q , respectively. The quadrupole operators (Q_{η}^I for an impurity; Q_{η}^c for an electron) are defined as

$$\begin{aligned} \{Q_{\eta}, \eta = 1, \dots, 5\} \\ = \{S_y S_z + S_z S_y, S_z S_x + S_x S_z, S_x S_y + S_y S_x, \\ S_x^2 - S_y^2, (2S_z^2 - S_x^2 - S_y^2)/\sqrt{3}\}. \end{aligned} \quad (51)$$

The last term in eq. (50) introduces uniaxial (D_{4h} or D_{6h}) anisotropy to the impurity states, and $\Delta_{\text{CF}} (> 0)$ is taken to determine a singlet ground state here. For the $S^I = 1$ pseudo-spin, it is sufficient to consider the above dipoles and quadrupoles. We do not consider the anisotropy of each exchange coupling that usually exists in a realistic system, which does not affect the following argument.

On the other hand, we introduce some assumptions to electron states as follows. At impurity sites, partial waves of conduction electrons are represented by $S^c = 3/2$. This can be regarded as the $O_h \Gamma_8$ point-group basis in a cubic system. In general, actual conduction bands can include all four components of $S^c = 3/2$, and their mixing is expressed as

$$\psi^c = \hat{V} \psi_b, \quad \psi^c \equiv \begin{pmatrix} \psi_{3/2} \\ \psi_{1/2} \\ \psi_{-1/2} \\ \psi_{-3/2} \end{pmatrix}, \quad \psi_b \equiv \begin{pmatrix} \psi_{+\uparrow} \\ \psi_{+\downarrow} \\ \psi_{-\uparrow} \\ \psi_{-\downarrow} \end{pmatrix}, \quad (52)$$

where each element in the transformation matrix \hat{V} is given by the overlap of local orbital and band wave functions such as $\langle S_z^c | \mu \sigma \rangle$ ($\mu = \pm; \sigma = \uparrow, \downarrow$). To examine the orbital roles in the superconductivity, we consider here the simplest case in which two ($\pm 3/2$) of the orbital components enter the $+$ band and the other two ($\pm 1/2$) enter the $-$ band. In the above \hat{V} , we assume that $\langle 3/2 | + \downarrow \rangle = \langle 1/2 | - \uparrow \rangle = \langle -1/2 | - \downarrow \rangle = \langle -3/2 | + \uparrow \rangle = V_0$ and that the other matrix elements vanish:

$$\hat{V} = V_0 \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \end{pmatrix}. \quad (53)$$

Such a one to one correspondence clarifies the connection between the $S^c = 3/2$ pseudo-spin space and the $\text{SU}(2)$ spin \otimes $\text{SU}(2)$ band space, and the scattering matrices are expressed simply by eqs. (B-9) and (B-10). Although this simplification overestimates interband scattering compared with intraband scattering, it helps us examine what types of interband correlations are relevant to the relative signs of order parameters and how

intraband scattering modifies their relative amplitudes.

For the superconducting order parameters, we consider both the s_{++} wave ($\Delta_+ = \Delta_-$) and the s_{\pm} wave ($\Delta_+ = -\Delta_-$). Since we neglect any correlations between the two bands except for the impurity scattering, the local correlations directly affect the relative signs of order parameters together with their amplitudes. This is justified when the impurity effect is more relevant than any other interband correlation such as an interband Coulomb interaction. We respectively express the s_{++} -wave and s_{\pm} -wave states as

$$\hat{\Delta}_A = \Delta_A \hat{\rho}_2 \hat{\sigma}_2 \quad (s_{++} \text{ wave}), \quad (54)$$

$$\hat{\Delta}_B = \Delta_B \hat{\tau}_3 \hat{\rho}_2 \hat{\sigma}_2 \quad (s_{\pm} \text{ wave}), \quad (55)$$

with the order parameters Δ_A and Δ_B , respectively. The matrix for the order parameter is given by their combination as

$$\hat{\Delta} = \hat{\Delta}_A + \hat{\Delta}_B. \quad (56)$$

The relevant impurity scatterings for the singlet-doublet configuration are described in Appendix B. First, we examine properties of the dipolar and quadrupolar scatterings separately. Let us start from the dipolar (magnetic) scattering case where $J_S \neq 0$ and $J_Q = 0$ in eq. (50). Applying \mathcal{H}' in eq. (B.7) to calculate the self-energy in Fig. 1, we obtain

$$\begin{aligned} \hat{\Sigma}(i\omega_l) = & -n_{\text{imp}} T^2 \sum_{n \neq n'} \sum_{\omega_1 \omega_2} \frac{1}{i\omega_1 - \delta_n} \frac{1}{i\omega_2 - \delta_{n'}} (\sqrt{2})^2 \\ & \times \left(\frac{J_S}{2} \right)^2 \frac{1}{\Omega} \sum_{\mathbf{k}} (S_+^c \hat{G}_0 S_-^c + S_-^c \hat{G}_0 S_+^c), \end{aligned} \quad (57)$$

where $\hat{G}_0 \equiv \hat{G}_0(i\omega_l + i\omega_1 - i\omega_2, \mathbf{k})$. δ_1 (δ_2) corresponds to the energy level of the impurity singlet ground (doublet excited) state ($n, n' = 1, 2$) and $\delta_2 - \delta_1 = \Delta_{\text{CF}}$. The factor $(\sqrt{2})^2$ comes from the second-order process $S_+ S_-$ or $S_- S_+$ between the singlet and doublet states. Then, we derive a gap equation. As in eq. (31), the Green's function \hat{G}_0 consists of three parts: $i\omega_l$, $\epsilon_{\mathbf{k}} \hat{\rho}_3$, and $\hat{\Delta}$. The $\epsilon_{\mathbf{k}} \hat{\rho}_3$ term disappears after the summation over \mathbf{k} . The other two parts are transformed by $(S_+^c \hat{G}_0 S_-^c + S_-^c \hat{G}_0 S_+^c)$. For $\hat{\Delta}$,

$$\begin{aligned} S_+^c \hat{\Delta} S_-^c + S_-^c \hat{\Delta} S_+^c &= (5\Delta_A - 2\Delta_B) \hat{\rho}_2 \hat{\sigma}_2 + (-2\Delta_A - \Delta_B) \hat{\tau}_3 \hat{\rho}_2 \hat{\sigma}_2 \\ &= \Delta_A' \hat{\rho}_2 \hat{\sigma}_2 + \Delta_B' \hat{\tau}_3 \hat{\rho}_2 \hat{\sigma}_2. \end{aligned} \quad (58)$$

This means that the order parameters are transformed as

$$\begin{pmatrix} \Delta_A' \\ \Delta_B' \end{pmatrix} = \hat{\Lambda}_{\Delta}^S \begin{pmatrix} \Delta_A \\ \Delta_B \end{pmatrix}, \quad \hat{\Lambda}_{\Delta}^S = \begin{pmatrix} 5 & -2 \\ -2 & -1 \end{pmatrix}. \quad (59)$$

Similarly, the $i\omega_l$ part is

$$S_+^c i\omega_l S_-^c + S_-^c i\omega_l S_+^c = i\omega_l (5 - 2\hat{\tau}_3). \quad (60)$$

Since $\hat{\tau}_3$ is the Pauli matrix for the \pm band space, eq. (21)

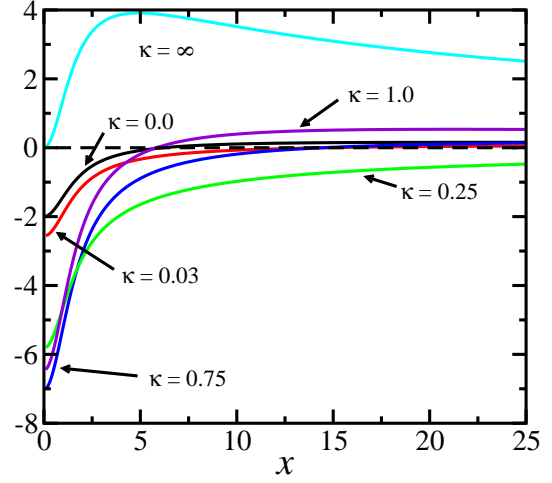


Fig. 3. (Color online) $x [= \Delta_{\text{CF}}/(2T_c)]$ dependence of the highest eigenvalue of the matrix $\bar{\tau}_{12} \hat{\Lambda}(x)$ for T_c . The plot is shown for fixed $\kappa = J_Q^2/J_S^2$ values.

is obtained as

$$\hat{\lambda}_{\omega}^S = \begin{pmatrix} 3 & 0 \\ 0 & 7 \end{pmatrix}, \quad (61)$$

for $X = S$ and $\xi = \omega$. Then, eq. (22) yields

$$\hat{\Lambda}_{\omega}^S = \hat{U}^{-1} \hat{\lambda}_{\omega}^S \hat{U} = \begin{pmatrix} 5 & -2 \\ -2 & 5 \end{pmatrix}. \quad (62)$$

Both $\hat{\Lambda}_{\Delta}^S$ and $\hat{\Lambda}_{\omega}^S$ can be divided into interband and intraband scattering parts as follows:

$$\begin{aligned} \hat{\Lambda}_{\Delta}^S &= \begin{pmatrix} 3 & 0 \\ 0 & -3 \end{pmatrix} + \begin{pmatrix} 2 & -2 \\ -2 & 2 \end{pmatrix}, \\ \hat{\Lambda}_{\omega}^S &= \begin{pmatrix} 3 & 0 \\ 0 & 3 \end{pmatrix} + \begin{pmatrix} 2 & -2 \\ -2 & 2 \end{pmatrix}. \end{aligned} \quad (63)$$

If the intraband contribution, the second matrix on the right-hand side of each equation, is removed, the interband contribution results in the T_c enhancement for the s_{\pm} state, as discussed in §2.3.

In the same manner, the above argument is applied to the quadrupolar (nonmagnetic) scattering case where $J_S = 0$ and $J_Q \neq 0$ in eq. (50). For the $\hat{\Delta}$ and $i\omega_l$ parts in the self-energy,

$$Q_+^c \hat{\Delta} Q_-^c + Q_-^c \hat{\Delta} Q_+^c = -12\Delta_A \hat{\rho}_2 \hat{\sigma}_2 + 12\Delta_B \hat{\tau}_3 \hat{\rho}_2 \hat{\sigma}_2, \quad (64)$$

$$Q_+^c i\omega_l Q_-^c + Q_-^c i\omega_l Q_+^c = 12i\omega_l, \quad (65)$$

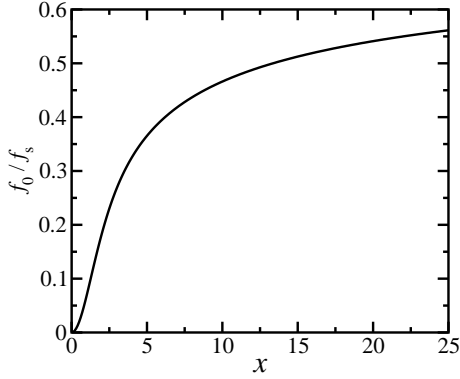
respectively, and we obtain

$$\hat{\Lambda}_{\Delta}^Q = \begin{pmatrix} -12 & 0 \\ 0 & 12 \end{pmatrix}, \quad \hat{\Lambda}_{\omega}^Q = \begin{pmatrix} 12 & 0 \\ 0 & 12 \end{pmatrix}. \quad (66)$$

These lead to the T_c enhancement for the s_{++} -wave state.

Next, we see the more generic treatment combining both magnetic (S) and nonmagnetic (Q) scattering terms as

$$\begin{aligned} \bar{\tau}_{12} \hat{\Lambda}(x) &= \cos \zeta \left[f_{\Delta}(x) \hat{\Lambda}_{\Delta}^S + f_{\omega}(x) \hat{\Lambda}_{\omega}^S \right] \\ &\quad + \sin \zeta \left[f_{\Delta}(x) \hat{\Lambda}_{\Delta}^Q + f_{\omega}(x) \hat{\Lambda}_{\omega}^Q \right] \end{aligned}$$

Fig. 4. Ratio f_0/f_s as a function of $x = \Delta_{CF}/(2T_c)$.

$$= \begin{pmatrix} [-5f_s(x) \cos \zeta & 2f_s(x) \cos \zeta \\ +12f_0(x) \sin \zeta] & \{[3f_0(x) - 2f_s(x)] \cos \zeta \\ 2f_s(x) \cos \zeta & -12f_s(x) \sin \zeta \} \end{pmatrix}, \quad (67)$$

in eq. (24), where

$$\bar{\tau}_{12} = \frac{\tau_{12}^S \tau_{12}^Q}{\sqrt{(\tau_{12}^S)^2 + (\tau_{12}^Q)^2}}, \quad \tan \zeta = \frac{J_Q^2}{J_S^2} \equiv \kappa, \quad (68)$$

and the lifetime τ_{12}^S (τ_{12}^Q) is introduced for the magnetic (nonmagnetic) scattering. The highest eigenvalue of $\bar{\tau}_{12}\hat{\Lambda}$ determines the quantity of

$$\frac{8T_c}{\pi} \bar{\tau}_{12} \log \frac{T_c}{T_{c0}}, \quad (69)$$

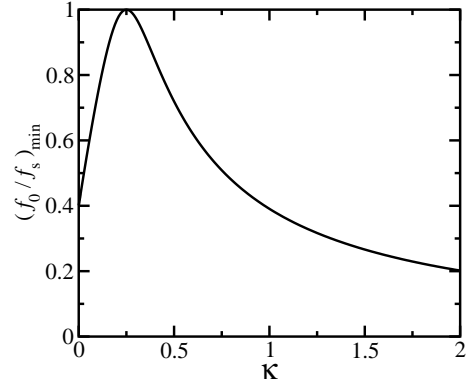
and its x dependence is shown in Fig. 3. The T_c enhancement is obtained for its positive value, which holds at $x > 6.2$ for $\kappa = 0$ and at $x > 5.8$ for $\kappa = 1.0$. In the presence of only nonmagnetic scattering for $\kappa = \infty$, T_c is enhanced in the entire $x > 0$ range. The T_c suppression, found for a small x or $\kappa \simeq 0.25$, is due to the competition between the magnetic and nonmagnetic exchange scatterings and to the depairing effect by the intraband scattering. Since $f_0/f_s < 1$, the condition for a positive value of eq. (69) is given by

$$(-5f_s + 12\kappa f_0)(3f_0 - 2f_s - 12\kappa f_s) - (2f_s)^2 < 0, \quad (70)$$

the solution of which determines the minimum f_0/f_s as a function of κ :

$$\left(\frac{f_0}{f_s}\right)_{\min} = \frac{1}{24\kappa} [(48\kappa^2 + 8\kappa + 5) - \sqrt{(48\kappa^2 + 8\kappa + 5)^2 - 96\kappa(10\kappa + 1)}]. \quad (71)$$

The x dependence of f_0/f_s and the κ dependence of $(f_0/f_s)_{\min}$ are shown in Figs. 4 and 5, respectively. At both $\kappa = 0.03$ and $\kappa = 0.75$, for instance, eq. (71) takes almost the same value, $\simeq 0.51$, which gives the minimum $x \simeq 14.5$ for T_c enhancement, as shown in Fig. 3. The maximum at $\kappa = 0.25$ in Fig. 5 indicates that there is no T_c enhancement for any finite crystal-field level splitting, implying that T_c is always suppressed by the competi-

Fig. 5. κ ($= J_Q^2/J_S^2$) dependence of the minimum of the ratio f_0/f_s for T_c enhancement.

tion between the magnetic and nonmagnetic scattering effects. We also find that κ determines the relative signs of the two order parameters: $\Delta_+\Delta_- < 0$ for $\kappa < 0.25$ and $\Delta_+\Delta_- > 0$ for $\kappa > 0.25$. The combination of $\hat{\Delta}_A$ (s_{++} wave) and $\hat{\Delta}_B$ (s_{\pm} wave) is caused by the intraband scattering effect in the $-$ band, due to the off-diagonal elements in $\hat{\Lambda}(x)$, which leads to $|\Delta_-| < |\Delta_+|$ in the vicinity of T_c . At $\kappa = 0.25$, $\Delta_- = 0$ ($\Delta_A = \Delta_B$) means that only one band ($+$ band) is superconducting with T_c suppression.

The above argument is based on a rather artificial assumption about the local band character in eq. (53). More generic treatment of \hat{V} in eq. (52) provides us with various scattering effects on T_c . This point is considered for the singlet-triplet configuration discussed below.

3.3 Singlet-triplet configuration

The singlet-triplet configuration is realized for a non-Kramers ion in an O_h crystal field environment like the Pr^{3+} or U^{4+} f^2 low-lying states in heavy-fermion materials. For the strong spin-orbit coupling, the most relevant local f -electron states are described by the $j = 5/2$ angular momentum. Then, we consider only the exchange coupling between the impurity states and the $j = 5/2$ electrons hybridized with conduction bands. We assume here that the Γ_8 and Γ_7 partial waves (see Appendix C) are transferred independently to the $+$ and $-$ bands, respectively. In terms of eq. (C.6) for both Γ_8 and Γ_7 , $\psi_m = (\psi_{m1\uparrow} \ \psi_{m1\downarrow} \ \psi_{m2\uparrow} \ \psi_{m2\downarrow} \ \psi_{m3\uparrow} \ \psi_{m3\downarrow})^t$ is combined with $\psi_b = (\psi_{+\uparrow} \ \psi_{+\downarrow} \ \psi_{-\uparrow} \ \psi_{-\downarrow})^t$ for the bands. This is expressed by $\psi_m = \hat{V}\psi_b$:

$$\hat{V} = \begin{pmatrix} v_+u_{1\uparrow} & v_+v_{1\uparrow} & 0 & 0 \\ v_+v_{1\downarrow} & v_+u_{1\downarrow} & 0 & 0 \\ v_+u_{2\uparrow} & v_+v_{2\uparrow} & 0 & 0 \\ v_+v_{2\downarrow} & v_+u_{2\downarrow} & 0 & 0 \\ 0 & 0 & v_- & 0 \\ 0 & 0 & 0 & v_- \end{pmatrix}. \quad (72)$$

Here, v_{\pm} represents the hybridization amplitude of the f -orbitals and the $\mu = \pm$ band, respectively, at the impurity sites;

$$\begin{aligned} u_{i\uparrow} &= \langle m_i \uparrow | + \uparrow \rangle, & v_{i\uparrow} &= \langle m_i \uparrow | + \downarrow \rangle, \\ v_{i\downarrow} &= \langle m_i \downarrow | + \uparrow \rangle, & u_{i\downarrow} &= \langle m_i \downarrow | + \downarrow \rangle \end{aligned} \quad (73)$$

represent the impurity site overlaps of the wave functions $\psi_{m_i, \sigma}$ ($i = 1, 2$) and $\psi_{+, \sigma}$. We only simplify the connection between the m_3 orbital and the $-$ band.

In Appendix C, the relevant impurity scatterings are described for the singlet-triplet configuration $\Gamma_1 \oplus \Gamma$ ($\Gamma = \Gamma_4, \Gamma_5$). For \mathcal{H}' in eq. (C-23), the self-energy in Fig. 1 is obtained as

$$\begin{aligned} \hat{\Sigma}^\Gamma(i\omega_l) = & -n_{\text{imp}} T^2 \sum_{n \neq n'} \sum_{\omega_1 \omega_2} \frac{1}{i\omega_1 - \delta_n} \frac{1}{i\omega_2 - \delta_{n'}} \\ & \times \sum_{X=S, Q} (J_X^\Gamma)^2 \frac{1}{\Omega} \sum_{\mathbf{k}} \left\{ X_z^{c, \Gamma} \hat{G}_0 X_z^{c, \Gamma} \right. \\ & \left. + \frac{1}{2} \left[X_+^{c, \Gamma} \hat{G}_0 X_-^{c, \Gamma} + X_-^{c, \Gamma} \hat{G}_0 X_+^{c, \Gamma} \right] \right\} \\ & [\hat{G}_0 \equiv \hat{G}_0(i\omega_l + i\omega_1 - i\omega_2, \mathbf{k})]. \end{aligned} \quad (74)$$

Here, δ_1 (δ_2) corresponds to the energy level of the impurity singlet ground (triplet excited) state ($n, n' = 1, 2$). For the gap equation in eq. (24), the transformation to $\hat{\Delta}$ in eq. (56),

$$X_z^{c, \Gamma} \hat{\Delta} X_z^{c, \Gamma} + \frac{1}{2} (X_+^{c, \Gamma} \hat{\Delta} X_-^{c, \Gamma} + X_-^{c, \Gamma} \hat{\Delta} X_+^{c, \Gamma}), \quad (75)$$

leads to

$$\hat{\Lambda}_\Delta^S = (-1) \hat{\Lambda}_\Delta^Q = \frac{3}{8} \sum_{i=1}^2 (u_{i\uparrow} u_{i\downarrow} - v_{i\uparrow} v_{i\downarrow}) \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}, \quad (76)$$

in both $\Gamma = \Gamma_4$ and $\Gamma = \Gamma_5$ cases. For the derivation, we use $u_{i\uparrow} u_{i\downarrow} = u_{i\uparrow}^* u_{i\downarrow}^*$ and $v_{i\uparrow} v_{i\downarrow} = v_{i\uparrow}^* v_{i\downarrow}^*$ since the $m_{i\uparrow}$ and $m_{i\downarrow}$ local electrons are the time reversal partners. In the same manner, for both Γ_4 and Γ_5 ,

$$X_z^{c, \Gamma} i\omega_l X_z^{c, \Gamma} + \frac{1}{2} (X_+^{c, \Gamma} i\omega_l X_-^{c, \Gamma} + X_-^{c, \Gamma} i\omega_l X_+^{c, \Gamma}) \quad (77)$$

gives

$$\hat{\Lambda}_\omega^S = \hat{\Lambda}_\omega^Q = \frac{3}{16} \sum_{i=1}^2 \sum_{\sigma=\uparrow, \downarrow} (u_{i\sigma}^* u_{i\sigma} + v_{i\sigma}^* v_{i\sigma}) \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}. \quad (78)$$

Equation (76) implies the competition between the magnetic (S) and nonmagnetic (Q) scattering effects for T_c enhancement. Which has the higher T_c , the s_{++} wave or the s_{\pm} wave, depends on whether the sign of $(u_{i\uparrow} u_{i\downarrow} - v_{i\uparrow} v_{i\downarrow})$ is positive or negative, respectively. In realistic systems, both magnetic and nonmagnetic scatterings coexist. In the present case, we can calculate the coupling constants, J_S^Γ and J_Q^Γ , based on the Anderson model including the $j = 5/2$ electron exchange scattering due to a single impurity in the f^2 configuration,³⁰⁾ and obtain the ratio as $|J_Q^\Gamma|/|J_S^\Gamma| = 1/3$.³¹⁾ This means that the magnetic interband scattering dominates the T_c enhancement for the singlet-triplet configuration. A more detailed discussion is given below.

4. Pr Impurity Effect in $\text{LaOs}_4\text{Sb}_{12}$ Superconductor

The Pr^{3+} f^2 configuration is a good candidate for raising T_c if Pr can be embedded in a multiband su-

perconductor. In fact, for the skutterudite superconductor $\text{La}_{1-x}\text{Pr}_x\text{Os}_4\text{Sb}_{12}$, the Pr singlet-triplet configuration may be relevant to T_c enhancement in $\text{LaOs}_4\text{Sb}_{12}$.²⁵⁾ Here, we show an attempt to apply the above argument in this case. The most intriguing feature of the skutterudite compounds is that each rare-earth ion is located at the center of the pnictogen cage (Sb_{12}) having the $a_u(xyz)$ and $t_u(x, y, z)$ molecular orbitals. It is considered that the Pr f -electron states hybridize with the conduction bands via these orbitals. For a strong spin-orbit coupling, the a_u electrons have the O_h Γ_7 symmetry and transfer directly to the m_3 electron state named in eq. (C-6). On the other hand, the t_u electrons with the O_h Γ_8 symmetry mix with both m_1 and m_2 states as³²⁾

$$|m_1, \uparrow\rangle \leftrightarrow \frac{1}{\sqrt{2}}(|x, \downarrow\rangle - i|y, \downarrow\rangle), \quad (79)$$

$$|m_1, \downarrow\rangle \leftrightarrow -\frac{1}{\sqrt{2}}(|x, \uparrow\rangle + i|y, \uparrow\rangle), \quad (80)$$

$$|m_2, \uparrow\rangle \leftrightarrow \frac{1}{\sqrt{3}} \left[\sqrt{2}|z, \uparrow\rangle - \frac{1}{\sqrt{2}}(|x, \downarrow\rangle + i|y, \downarrow\rangle) \right], \quad (81)$$

$$|m_2, \downarrow\rangle \leftrightarrow \frac{1}{\sqrt{3}} \left[\sqrt{2}|z, \downarrow\rangle + \frac{1}{\sqrt{2}}(|x, \uparrow\rangle - i|y, \uparrow\rangle) \right]. \quad (82)$$

We here consider two conduction bands, one of which is a_u -dominant and the other is t_u -dominant. We assume that both are combined with each other only through interband electron scattering. In the present case, the most relevant is the Pr impurity scattering due to the hybridization effect with the bands. Then, we can use the transformation in eq. (72) for mixing f -electron states with the t_u -dominant band ($+$ band) and the a_u -dominant band ($-$ band). Choosing the local $t_u(x, y, z)$ component that mainly contributes to the $+$ band and taking their onsite overlaps arbitrarily as

$$\langle x|+\rangle : \langle y|+\rangle : \langle z|+\rangle = \sin \theta \cos \phi : \sin \theta \sin \phi : \cos \theta, \quad (83)$$

we have

$$u_{1\uparrow} = u_{1\downarrow} = 0,$$

$$v_{1\uparrow} = (1/\sqrt{2}) \sin \theta e^{i\phi}, \quad v_{1\downarrow} = -(1/\sqrt{2}) \sin \theta e^{-i\phi},$$

$$u_{2\uparrow} = u_{2\downarrow} = (\sqrt{2/3}) \cos \theta,$$

$$v_{2\uparrow} = -(1/\sqrt{6}) \sin \theta e^{-i\phi}, \quad v_{2\downarrow} = (1/\sqrt{6}) \sin \theta e^{i\phi} \quad (84)$$

Substituting them in eqs. (76) and (78), we obtain

$$\hat{\Lambda}_\Delta^S = (-1) \hat{\Lambda}_\Delta^Q = \frac{1}{4} \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}, \quad (85)$$

$$\hat{\Lambda}_\omega^S = \hat{\Lambda}_\omega^Q = \frac{1}{4} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}. \quad (86)$$

In the gap equation (24), we have

$$\begin{aligned} \hat{\Lambda}(x) = & \frac{1}{4\tau_{12}^S} \begin{pmatrix} f_0(x) & 0 \\ 0 & -f_s(x) \end{pmatrix} \\ & + \frac{1}{4\tau_{12}^Q} \begin{pmatrix} -f_s(x) & 0 \\ 0 & f_0(x) \end{pmatrix}. \end{aligned} \quad (87)$$

In the real system, we must consider the T_h symmetry that combines the Pr O_h Γ_4 and Γ_5 triplet states as^{31, 33, 34)}

$$|\Gamma_4^{(2)}\eta\rangle = \sqrt{1-d^2}|\Gamma_5\eta\rangle + d|\Gamma_4\eta\rangle \quad (\eta = +, 0, -), \quad (88)$$

where d ($0 < d < 1/\sqrt{2}$) represents the deviation from the O_h symmetry. In the above calculation of the self-energy, we usually have additional terms, namely,

$$\begin{aligned} & \left[X_{z,\Gamma_4}^c \hat{\Delta} X_{z,\Gamma_5}^c + \frac{1}{2} (X_{+,\Gamma_4}^c \hat{\Delta} X_{-,\Gamma_5}^c + X_{-,\Gamma_4}^c \hat{\Delta} X_{+,\Gamma_5}^c) \right] \\ & + (\Gamma_4 \leftrightarrow \Gamma_5) \quad (X^c = s, q), \end{aligned} \quad (89)$$

which vanish in this case. They also vanish when $\hat{\Delta}$ is replaced with $i\omega$. If the a_u band hybridizes with the f -orbitals more strongly than the t_u band, which means $v_- \gg v_+$ here, the impurity interband scattering enhances T_c for a finite crystal-field splitting $x [= (\delta_2 - \delta_1)/(2T_c)]$, satisfying either $f_0/f_s > \tau_{12}^S/\tau_{12}^Q$ or $f_0/f_s > \tau_{12}^Q/\tau_{12}^S$. For the former, the T_c enhancement is possible in the s_{++} -wave state, and a higher T_c can be realized as the magnetic scattering becomes more dominant. In §3.3, we have mentioned that $|J_Q|/|J_S| = 1/3$ ($\tau_{12}^S/\tau_{12}^Q = 1/9$) is satisfied for O_h . It also holds for T_h ,³¹⁾ so that the gap equation chooses the s_{++} wave for the T_c enhancement. One may think that the quadrupolar scattering is the most relevant if d is small in eq. (88), since the Γ_1 - Γ_5 interchange dominates the exchange scattering. For the Γ_5 scattering type, however, the octupolar scattering cannot be neglected in the multiorbital exchange owing to the hybridization of f -electrons with the conduction bands. Thus, the magnetic scattering can contribute to the T_c enhancement for the Γ_1 - $\Gamma_4^{(2)}$ configuration in a multiband system. Our result indicates that the s_{++} -wave state is favorable for the $\text{La}_{1-x}\text{Pr}_x\text{Os}_4\text{Sb}_{12}$ superconductivity if the multiband picture is applicable and the Pr or Sb₁₂ site local orbital symmetries reflect in the bands.

Finally, we mention the effect of intraband scattering neglected in the above argument where $v_- \gg v_+$ is assumed for the hybridization amplitudes. If the m_1 - m_2 scattering terms in eqs. (C·17) and (C·18) are considered in calculating the self-energy for the Γ_5 nonmagnetic scattering type, a correction term,

$$C_v \frac{1}{\tau_{12}^Q} f_0(x) \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \quad \left(C_v \sim \frac{v_+^2}{v_-^2} \right), \quad (90)$$

is added on the right-hand side in eq. (87). It assists the T_c enhancement, which resembles the effect of inelastic nonmagnetic scattering impurities in single-band s -wave superconductors.

5. Conclusion

We have studied inelastic (dynamical) impurity scattering effects on T_c enhancement in the two-band superconducting states, s_{++} wave and s_{\pm} wave. The key is to check the sign change of the order parameters in the self-energy corresponding to the second order of the scattering process. We solve a gap equation, where both

the s_{++} wave and s_{\pm} wave are combined by impurity scattering, and find out the possible atomic structure of the impurity that increases T_c . For the T_c enhancement, the crystal-field ground state must be a singlet or a nonmagnetic doublet. If not, magnetic impurities will always cause T_c suppression. For the s_{\pm} wave, it is necessary for elastic (nonmagnetic) scattering to be relatively small. In the singlet-singlet configuration, we can easily determine what type of magnetic interband scattering contributes to pairing interaction. This simple analysis is very useful for determining a scattering type for the T_c enhancement among multiorbital interaction terms when we consider such a complicated atomic structure as the f^n configuration. Here, we have discussed the singlet-doublet and singlet-triplet configurations. We find that the T_c of either the s_{++} -wave or s_{\pm} -wave state can be enhanced by the dynamical magnetic or nonmagnetic impurity interband scattering for a larger crystal-field splitting of impurity ground and excited states, while T_c is suppressed if both scattering strengths are comparable. Whether T_c is enhanced or not also depends on how the local electron states hybridize with the two bands. We show a case of T_c enhancement in the s_{++} wave by magnetic interband scattering due to the singlet-triplet configuration. This result may give useful information on a multiband picture of the $\text{La}_{1-x}\text{Pr}_x\text{Os}_4\text{Sb}_{12}$ superconductivity. In fact, the connection between the La-rich and Pr-rich superconductors is left to be clarified as well as the symmetry of the latter order parameter.³⁵⁾

In the above argument, we have assumed weak scattering impurities. Strictly speaking, dynamical scattering effects should be investigated as a Kondo problem. It was shown theoretically in normal metallic cases that the impurity exchange scattering strength is renormalized to be weaker with the decrease in temperature since the crystal-field singlet competes with the Kondo-singlet formation.^{29, 36–38)} This holds even for a small crystal-field splitting of the singlet ground and excited multiplet states. Thus, our results shown here are valid for the T_c enhancement due to the impurity scattering.

Throughout the paper, we focus on the hybridization between local orbitals and conduction electron states. For most of the f -electron systems, this may be more relevant than the admixture of orbitals formed by intersite electron hopping that we have neglected here. Our treatment is more practical since the latter contribution can be included effectively in the hybridization.

The possibility of the s_{\pm} -wave state has been the subject of debate for high- T_c superconductors with FeAs layers. It is pointed out that the Fe d -orbitals contribute to the disconnected Fermi surfaces and the orbital degrees of freedom play an important role in pairing interaction.⁸⁾ The interband Coulomb interactions may be relevant for the high T_c of this multiband superconductivity,^{28, 39, 40)} the roles of which are analogous to those of the local correlations in the f -electron systems we have considered here.

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Appendix A: Connection between the s_{\pm} -Wave and Conventional s -Wave Superconductors

We attempt to apply the unitary transformation

$$\begin{pmatrix} \psi_{+, \sigma} \\ \psi_{-, \sigma} \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix} \begin{pmatrix} \psi_{M\sigma} \\ \psi_{-M\sigma} \end{pmatrix} \quad (\text{A.1})$$

to the band basis, where M is a natural number. Using this new basis set, $\psi_M = (\psi_{M\uparrow} \ \psi_{M\downarrow} \ \psi_{-M\uparrow} \ \psi_{-M\downarrow})^t$, \hat{U}_{mn}^z in eq. (40) is transformed as

$$\hat{U}_{mn}^z \rightarrow -M_{mn}^z \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}_{M \text{ space}}. \quad (\text{A.2})$$

If the number M is regarded as an orbital component, this matrix indicates a quadrupole type of scattering. In fact, $\psi_{M=1}$ corresponds directly to $\psi_{j=3/2}$ in §3.1. In this case, the matrix in eq. (A.2) is expressed by $(2j_z^2 - j_x^2 - j_y^2)$.

On the other hand, for the conventional single-band s -wave superconductivity, the pairing Hamiltonian is given by

$$\mathcal{H}_{\Delta} = - \sum_{\mathbf{k}} \Delta \left(c_{\mathbf{k}\uparrow}^{\dagger} c_{-\mathbf{k}\downarrow}^{\dagger} + c_{-\mathbf{k}\downarrow} c_{\mathbf{k}\uparrow} \right). \quad (\text{A.3})$$

After applying spherical expansion to the operators as

$$c_{\mathbf{k}\sigma} = \sum_{LM} i^{-L} \frac{(6\pi)^{1/2}}{kR} Y_{LM}(\Omega_{\mathbf{k}}) c_{kLM\sigma}, \quad (\text{A.4})$$

where R is the radius of the system, we rewrite the Hamiltonian (A.3) as

$$\begin{aligned} \mathcal{H}_{\Delta} = & - \sum_{\mathbf{k}} \sum_{L,M \geq 0} (-1)^M \Delta \\ & \times \left(c_{kLM\uparrow}^{\dagger} c_{kL,-M\downarrow}^{\dagger} + c_{kL,-M\downarrow} c_{kLM\uparrow} \right). \end{aligned} \quad (\text{A.5})$$

This orbital component M can correspond to M in eq. (A.1) directly. The pairing interaction works between the electrons with the different orbitals denoted by $\pm M$. Let us fix L and restrict the orbitals to a pair of $\pm M$. If $\psi_{M\sigma}$ is transformed to $\psi_{\mu\sigma}$ using eq. (A.1), eq. (A.5) is reduced to

$$\mathcal{H}_{\Delta} = - \sum_{\mu=\pm} \sum_{\mathbf{k}} (-1)^M \mu \Delta \left(c_{k\mu\uparrow}^{\dagger} c_{k\mu\downarrow}^{\dagger} + c_{k\mu\downarrow} c_{k\mu\uparrow} \right). \quad (\text{A.6})$$

It represents s_{\pm} -wave pairing in the two orbitals connected to the μ bands.

Thus the spin-dependent interband scattering in eq. (40) in a two-band s_{\pm} -wave superconductor can be mapped to the quadrupole type of scattering in eq. (A.2) in a single-band s -wave superconductor. Both cases give

rise to the T_c enhancement if the electron scattering interchanges the impurity low-lying states with a finite crystal-field splitting.

Appendix B: Exchange Matrices for Singlet-Doublet Configuration

At low temperatures, the most relevant terms in eq. (50) are electron scatterings with interchange between the local ground and excited states given by

$$J_S [S_x^I S_x^c + S_y^I S_y^c] + J_Q [Q_1^I Q_1^c + Q_2^I Q_2^c]. \quad (\text{B.1})$$

Using $S_{\pm} = S_x \pm iS_y$ and $Q_{\pm} = \pm iQ_1 + Q_2$, it is rewritten as

$$\frac{J_S}{2} [S_+^I S_-^c + S_-^I S_+^c] + \frac{J_Q}{2} [Q_+^I Q_-^c + Q_-^I Q_+^c]. \quad (\text{B.2})$$

By denoting $S_z^I = 0$ (the impurity ground state) and $S_z^I = 1, -1$ (the impurity excited states) by $|1\rangle$, $|2\rangle$, and $|3\rangle$, respectively, the $(S_{\pm}^I)_{mn}$ and $(Q_{\pm}^I)_{mn}$ ($m, n = 1, 2, 3$) matrix expressions are given as

$$S_+^I = S_-^{I\dagger} = \begin{pmatrix} 0 & 0 & \sqrt{2} \\ \sqrt{2} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \quad (\text{B.3})$$

$$Q_+^I = Q_-^{I\dagger} = \begin{pmatrix} 0 & 0 & -\sqrt{2} \\ \sqrt{2} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}. \quad (\text{B.4})$$

For the $S^c = 3/2$ states, the operators $S_+^c = S_-^{c\dagger}$ and $Q_+^c = Q_-^{c\dagger}$ are expressed by

$$\psi^{c\dagger} S_+^c \psi^c = \psi^{c\dagger} \begin{pmatrix} 0 & \sqrt{3} & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & \sqrt{3} \\ 0 & 0 & 0 & 0 \end{pmatrix} \psi^c, \quad (\text{B.5})$$

$$\psi^{c\dagger} Q_+^c \psi^c = \psi^{c\dagger} \begin{pmatrix} 0 & 2\sqrt{3} & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -2\sqrt{3} \\ 0 & 0 & 0 & 0 \end{pmatrix} \psi^c. \quad (\text{B.6})$$

Following eq. (26), we examine the low-temperature physics using the impurity interaction Hamiltonian

$$\begin{aligned} \mathcal{H}' = & \sum_{X=S,Q} \sum_{\mathbf{R}_{\gamma}} \sum_{mn} \int d\mathbf{r} a_{\gamma m}^{\dagger} a_{\gamma n} \delta(\mathbf{r} - \mathbf{R}_{\gamma}) \\ & \times \Psi^{\dagger}(\mathbf{r}) \frac{J_X}{2} (X_{+,mn}^I X_-^c + X_{-,mn}^I X_+^c) \Psi(\mathbf{r}). \end{aligned} \quad (\text{B.7})$$

Here, Ψ is an eight-dimensional vector for conduction electrons that is obtained by extending ψ_b in eq. (52) to the particle-hole space as

$$\Psi = \begin{pmatrix} \Psi_+ \\ \Psi_- \end{pmatrix}, \quad \Psi^{\dagger} = \begin{pmatrix} \Psi_+^{\dagger} & \Psi_-^{\dagger} \end{pmatrix}, \quad (\text{B.8})$$

where Ψ_{μ} ($\mu = +, -$) is defined in eq. (28). Through \hat{V} in eq. (53) in this extended space (Pauli matrices $\hat{\sigma}$ for spin, $\hat{\rho}$ for particle hole, and $\hat{\tau}$ for band), the above

electron scattering matrices are rewritten as

$$S_+^c = \frac{\sqrt{3}}{2}\hat{\tau}_1(\hat{\rho}_3\hat{\sigma}_1 - i\hat{\sigma}_2) + \frac{1}{2}(1 - \hat{\tau}_3)(\hat{\rho}_3\hat{\sigma}_1 + i\hat{\sigma}_2), \quad (\text{B-9})$$

$$Q_+^c = \sqrt{3}(i\hat{\tau}_2)(\hat{\sigma}_1 - i\hat{\rho}_3\hat{\sigma}_2), \quad (\text{B-10})$$

where $|V_0|^2$ has been omitted. One can see that S_\pm^c consists of the interband scattering τ_1 and intraband scattering $(1 - \hat{\tau}_3)$ terms. The former is comparable to $(\hat{U}^x - i\hat{U}^y)$ in eq. (32).

Appendix C: Exchange Matrices for Singlet-Triplet Configuration

On the basis of the $J = 4$ total angular momentum, the O_h singlet and triplet states are given by³⁴⁾

$$|\Gamma_1\rangle = \frac{\sqrt{30}}{12}(|4\rangle + |-4\rangle) + \frac{\sqrt{21}}{6}|0\rangle, \quad (\text{C-1})$$

$$\begin{cases} |\Gamma_4+\rangle = -\sqrt{\frac{1}{8}}|3\rangle - \sqrt{\frac{7}{8}}|1\rangle, \\ |\Gamma_4 0\rangle = \sqrt{\frac{1}{2}}(|4\rangle - |-4\rangle), \\ |\Gamma_4-\rangle = \sqrt{\frac{1}{8}}|3\rangle + \sqrt{\frac{7}{8}}|-1\rangle, \end{cases} \quad (\text{C-2})$$

$$\begin{cases} |\Gamma_5+\rangle = \sqrt{\frac{7}{8}}|3\rangle - \sqrt{\frac{1}{8}}|-1\rangle, \\ |\Gamma_5 0\rangle = \sqrt{\frac{1}{2}}(|2\rangle - |-2\rangle), \\ |\Gamma_5-\rangle = -\sqrt{\frac{7}{8}}|-3\rangle + \sqrt{\frac{1}{8}}|1\rangle. \end{cases} \quad (\text{C-3})$$

For the $j = 5/2$ local electrons, they are classified into the O_h symmetric states as³²⁾

$$\begin{cases} |\Gamma_{8,3/2}\rangle = -\sqrt{\frac{1}{6}}|3/2\rangle - \sqrt{\frac{5}{6}}|-5/2\rangle, \\ |\Gamma_{8,1/2}\rangle = |1/2\rangle, \\ |\Gamma_{8,-1/2}\rangle = -|-1/2\rangle, \\ |\Gamma_{8,-3/2}\rangle = \sqrt{\frac{1}{6}}|-3/2\rangle + \sqrt{\frac{5}{6}}|5/2\rangle, \end{cases} \quad (\text{C-4})$$

$$\begin{cases} |\Gamma_{7,1/2}\rangle = \sqrt{\frac{5}{6}}|-3/2\rangle - \sqrt{\frac{1}{6}}|5/2\rangle, \\ |\Gamma_{7,-1/2}\rangle = \sqrt{\frac{5}{6}}|3/2\rangle - \sqrt{\frac{1}{6}}|-5/2\rangle. \end{cases} \quad (\text{C-5})$$

In the following argument, we change their notations as

$$\begin{aligned} \Gamma_{8,-3/2} &\rightarrow (m_1, \uparrow), \quad \Gamma_{8,3/2} \rightarrow (m_1, \downarrow), \\ \Gamma_{8,1/2} &\rightarrow (m_2, \uparrow), \quad \Gamma_{8,-1/2} \rightarrow (m_2, \downarrow); \\ \Gamma_{7,1/2} &\rightarrow (m_3, \uparrow), \quad \Gamma_{7,-1/2} \rightarrow (m_3, \downarrow). \end{aligned} \quad (\text{C-6})$$

In the same manner as that in eq. (B-3) for an impurity, the magnetic coupling between the Γ_1 singlet ground (denoted by $|1\rangle$) and Γ ($= \Gamma_4, \Gamma_5$) triplet (+, 0 and - states denoted by $|2\rangle$, $|3\rangle$ and $|4\rangle$, respectively) excited states is expressed by the following matrices:³¹⁾

$$S_z^\Gamma = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad (\text{C-7})$$

$$S_+^\Gamma = S_-^{\Gamma\dagger} = \begin{pmatrix} 0 & 0 & 0 & \sqrt{2} \\ -\sqrt{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}. \quad (\text{C-8})$$

For nonmagnetic coupling,

$$Q_z^\Gamma = \begin{pmatrix} 0 & 0 & -i & 0 \\ 0 & 0 & 0 & 0 \\ i & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}, \quad (\text{C-9})$$

$$Q_+^\Gamma = Q_-^{\Gamma\dagger} = \begin{pmatrix} 0 & 0 & 0 & -\sqrt{2} \\ -\sqrt{2} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}. \quad (\text{C-10})$$

We note that the relative signs of the off-diagonal matrix elements are different between S_\pm^Γ (Q_\pm^Γ) for the pseudo-quartet and S_\pm^I (Q_\pm^I) for the $S^I = 1$ pseudo-spin given in eq. (B-3) [in eq. (B-4)]. The singlet-triplet interchange processes are mediated by the corresponding Γ_8 and Γ_7 electron scatterings as follows:³¹⁾

$$\psi_m^\dagger S_z^{\Gamma_4} \psi_m = \frac{1}{2}(\psi_{m_1\uparrow}^\dagger \psi_{m_3\uparrow} + \psi_{m_1\downarrow}^\dagger \psi_{m_3\downarrow}) + \text{H.c.}, \quad (\text{C-11})$$

$$\begin{aligned} \psi_m^\dagger S_+^{\Gamma_4} \psi_m &= \frac{1}{2}(-\psi_{m_1\uparrow}^\dagger \psi_{m_3\downarrow} + \psi_{m_3\uparrow}^\dagger \psi_{m_1\downarrow}) \\ &\quad + \frac{\sqrt{3}}{2}(\psi_{m_2\downarrow}^\dagger \psi_{m_3\uparrow} - \psi_{m_3\downarrow}^\dagger \psi_{m_2\uparrow}), \end{aligned} \quad (\text{C-12})$$

$$\psi_m^\dagger S_z^{\Gamma_5} \psi_m = \frac{1}{2}(\psi_{m_2\uparrow}^\dagger \psi_{m_3\uparrow} + \psi_{m_2\downarrow}^\dagger \psi_{m_3\downarrow}) + \text{H.c.}, \quad (\text{C-13})$$

$$\begin{aligned} \psi_m^\dagger S_+^{\Gamma_5} \psi_m &= \frac{1}{2}(-\psi_{m_2\uparrow}^\dagger \psi_{m_3\downarrow} + \psi_{m_3\uparrow}^\dagger \psi_{m_2\downarrow}) \\ &\quad + \frac{\sqrt{3}}{2}(-\psi_{m_1\downarrow}^\dagger \psi_{m_3\uparrow} + \psi_{m_3\downarrow}^\dagger \psi_{m_1\uparrow}), \end{aligned} \quad (\text{C-14})$$

$$\psi_m^\dagger Q_z^{\Gamma_4} \psi_m = -i\frac{1}{2}(\psi_{m_1\uparrow}^\dagger \psi_{m_3\uparrow} + \psi_{m_1\downarrow}^\dagger \psi_{m_3\downarrow}) + \text{H.c.}, \quad (\text{C-15})$$

$$\begin{aligned} \psi_m^\dagger Q_+^{\Gamma_4} \psi_m &= \frac{1}{2}(\psi_{m_1\uparrow}^\dagger \psi_{m_3\downarrow} + \psi_{m_3\uparrow}^\dagger \psi_{m_1\downarrow}) \\ &\quad + \frac{\sqrt{3}}{2}(-\psi_{m_2\downarrow}^\dagger \psi_{m_3\uparrow} - \psi_{m_3\downarrow}^\dagger \psi_{m_2\uparrow}), \end{aligned} \quad (\text{C-16})$$

$$\begin{aligned} \psi_m^\dagger Q_z^{\Gamma_5} \psi_m &= -i\left\{\frac{1}{2}(\psi_{m_2\uparrow}^\dagger \psi_{m_3\uparrow} + \psi_{m_2\downarrow}^\dagger \psi_{m_3\downarrow}) \right. \\ &\quad \left. + 2\sqrt{5}(\psi_{m_1\uparrow}^\dagger \psi_{m_2\uparrow} - \psi_{m_1\downarrow}^\dagger \psi_{m_2\downarrow})\right\} + \text{H.c.}, \end{aligned} \quad (\text{C-17})$$

$$\begin{aligned} \psi_m^\dagger Q_+^{\Gamma_5} \psi_m &= \frac{1}{2}(\psi_{m_2\uparrow}^\dagger \psi_{m_3\downarrow} + \psi_{m_3\uparrow}^\dagger \psi_{m_2\downarrow}) \\ &\quad + \frac{\sqrt{3}}{2}(\psi_{m_1\downarrow}^\dagger \psi_{m_3\uparrow} + \psi_{m_3\downarrow}^\dagger \psi_{m_1\uparrow}) \\ &\quad + 4\sqrt{5}(\psi_{m_1\uparrow}^\dagger \psi_{m_2\downarrow} - \psi_{m_2\uparrow}^\dagger \psi_{m_1\downarrow}). \end{aligned} \quad (\text{C-18})$$

In §3.3, we assume $v_- \gg v_+$ for the hybridization with the conduction band in eq. (72), i.e., we neglect the m_1 - m_2 orbital scattering terms in eqs. (C-17) and (C-18), whose contribution is small in the band scattering. Using

the transformation in eq. (72), the above multiorbital scattering operators are reduced to interband scattering operators. For the Γ_4 type,

$$\psi_b^\dagger s_z^{\Gamma_4} \psi_b = \psi_b^\dagger \frac{1}{2} \begin{pmatrix} 0 & 0 & u_{1\uparrow}^* & v_{1\downarrow}^* \\ 0 & 0 & v_{1\uparrow}^* & u_{1\downarrow}^* \\ u_{1\uparrow} & v_{1\uparrow} & 0 & 0 \\ v_{1\downarrow} & u_{1\downarrow} & 0 & 0 \end{pmatrix} \psi_b, \quad (\text{C}\cdot 19)$$

$$\psi_b^\dagger s_+^{\Gamma_4} \psi_b = \psi_b^\dagger \frac{1}{2} \begin{pmatrix} 0 & 0 & \sqrt{3}v_{2\downarrow}^* & -u_{1\uparrow}^* \\ 0 & 0 & \sqrt{3}u_{2\downarrow}^* & -v_{1\uparrow}^* \\ v_{1\downarrow} & u_{1\downarrow} & 0 & 0 \\ -\sqrt{3}u_{2\uparrow} & -\sqrt{3}v_{2\uparrow} & 0 & 0 \end{pmatrix} \psi_b, \quad (\text{C}\cdot 20)$$

$$\psi_b^\dagger q_z^{\Gamma_4} \psi_b = \psi_b^\dagger \left(-i\frac{1}{2}\right) \begin{pmatrix} 0 & 0 & u_{1\uparrow}^* & v_{1\downarrow}^* \\ 0 & 0 & v_{1\uparrow}^* & u_{1\downarrow}^* \\ -u_{1\uparrow} & -v_{1\uparrow} & 0 & 0 \\ -v_{1\downarrow} & -u_{1\downarrow} & 0 & 0 \end{pmatrix} \psi_b, \quad (\text{C}\cdot 21)$$

$$\psi_b^\dagger q_+^{\Gamma_4} \psi_b = \psi_b^\dagger \frac{1}{2} \begin{pmatrix} 0 & 0 & -\sqrt{3}v_{2\downarrow}^* & u_{1\uparrow}^* \\ 0 & 0 & -\sqrt{3}u_{2\downarrow}^* & v_{1\uparrow}^* \\ v_{1\downarrow} & u_{1\downarrow} & 0 & 0 \\ -\sqrt{3}u_{2\uparrow} & -\sqrt{3}v_{2\uparrow} & 0 & 0 \end{pmatrix} \psi_b, \quad (\text{C}\cdot 22)$$

where (v_+v_-) , which appears as the common factor in each matrix element, has been omitted. For the Γ_5 type, $s_z^{\Gamma_5}$ is obtained by switching the indices as $1 \leftrightarrow 2$ in the $s_z^{\Gamma_4}$ matrix, and $s_+^{\Gamma_5}$ by replacing $\sqrt{3} \rightarrow -\sqrt{3}$ in addition to switching $1 \leftrightarrow 2$ in the $s_+^{\Gamma_4}$ matrix; $q_z^{\Gamma_5}$ and $q_+^{\Gamma_5}$ are obtained from $q_z^{\Gamma_4}$ and $q_+^{\Gamma_4}$, respectively, in the same manner. We note that $s_z^{\Gamma_4}$ in eq. (C-19) is comparable to \hat{U}_{mn}^z in eq. (40) if $u_{1\uparrow} = -u_{1\downarrow} = u_{1\uparrow}^* = -u_{1\downarrow}^*$ and $v_{1\sigma} = 0$ are taken; $q_z^{\Gamma_4}$ in eq. (C-21) is comparable to \hat{U}_{mn} in eq. (46) for $u_{1\uparrow} = u_{1\downarrow} = u_{1\uparrow}^* = u_{1\downarrow}^*$ and $v_{1\sigma} = 0$. These scatterings, whichever is magnetic or nonmagnetic, contribute to T_c enhancement in the s_{\pm} -wave state. As discussed in §3.3, whether T_c is enhanced or suppressed by the interband scattering for the s_{\pm} wave and also for the s_{++} wave depends on the details of electron transfer, $u_{i\sigma}$ and $v_{i\sigma}$, between the f -orbitals and conduction bands at an impurity. As in eq. (B-7), we introduce the impurity interaction Hamiltonian for the singlet-triplet configuration for the Γ ($=\Gamma_4, \Gamma_5$) scattering,

$$\begin{aligned} \mathcal{H}'_{\Gamma} = & \sum_{X=S,Q} \sum_{\mathbf{R}_{\gamma}} \sum_{mn} \int d\mathbf{r} a_{\gamma m}^\dagger a_{\gamma n} \delta(\mathbf{r} - \mathbf{R}_{\gamma}) \\ & \times \Psi^\dagger(\mathbf{r}) J_X^\Gamma [X_{z,mn}^\Gamma X_z^{c,\Gamma} \\ & + \frac{1}{2} (X_{+,mn}^\Gamma X_-^{c,\Gamma} + X_{-,mn}^\Gamma X_+^{c,\Gamma})] \Psi(\mathbf{r}), \end{aligned} \quad (\text{C}\cdot 23)$$

where the band electron scattering operators

$$S^{c,\Gamma} = s^\Gamma, \quad Q^{c,\Gamma} = q^\Gamma, \quad (\text{C}\cdot 24)$$

are rewritten on the basis of the eight-dimensional vector Ψ in eq. (B-8).

- 1) Y. Kamihara, T. Watanabe, M. Hirano, and H. Hosono: J. Am. Chem. Soc. **130** (2008) 3296.
- 2) H. Takahashi, K. Igawa, K. Arii, Y. Kamihara, M. Hirano, and H. Hosono: Nature **453** (2008) 376.
- 3) A. Kawabata, S. C. Lee, T. Moyoshi, Y. Kobayashi, and M. Sato: J. Phys. Soc. Jpn. **77** (2008) 103704.
- 4) A. S. Sefat, R. Jin, A. McGuire, B. C. Sales, D. J. Singh, and D. Mandrus: Phys. Rev. Lett. **101** (2008) 117004.
- 5) A. Leithe-Jasper, W. Schnelle, C. Geibel, and H. Rosner: Phys. Rev. Lett. **101** (2008) 207004.
- 6) S. C. Lee, A. Kawabata, T. Moyoshi, Y. Kobayashi, and M. Sato: J. Phys. Soc. Jpn. **78** (2009) 043703.
- 7) M. Sato, Y. Kobayashi, S. C. Lee, H. Takahashi, E. Satomi, and Y. Miura: J. Phys. Soc. Jpn. **79** (2010) 014710.
- 8) For a progress report, K. Ishida, Y. Nakai, and H. Hosono: J. Phys. Soc. Jpn. **78** (2009) 062001.
- 9) J. Nagamatsu, N. Nakagawa, T. Muranaka, Y. Zenitani, and J. Akimitsu: Nature **410** (2001) 63.
- 10) J. Kortus, O. V. Dolgov, R. K. Kremer, and A. A. Golubov: Phys. Rev. Lett. **94** (2005) 027002.
- 11) M. Putti, P. Broto, M. Monni, E. Galleani d'Agliano, A. Sanna, and S. Massidda: Europhys. Lett. **77** (2007) 57005.
- 12) I. I. Mazin, D. J. Singh, M. D. Johannes, and M. H. Du: Phys. Rev. Lett. **101** (2008) 057003.
- 13) K. Kuroki, S. Onari, R. Arita, H. Usui, Y. Tanaka, H. Kontani, and H. Aoki: Phys. Rev. Lett. **101** (2008) 087004.
- 14) A. V. Chubukov, D. V. Efremov, and I. Eremin: Phys. Rev. B **78** (2008) 134512.
- 15) D. Parker, O. V. Dolgov, M. M. Korshunov, A. A. Golubov, and I. I. Mazin: Phys. Rev. B **78** (2008) 134524.
- 16) Y. Bang, H.-Y. Choi, and H. Won: Phys. Rev. B **79** (2009) 054529.
- 17) A. A. Golubov and I. I. Mazin: Phys. Rev. B **55** (1997) 15146.
- 18) G. Seyfarth, J. P. Brison, M.-A. Méasson, J. Flouquet, K. Izawa, Y. Matsuda, H. Sugawara, and H. Sato: Phys. Rev. Lett. **95** (2005) 107004.
- 19) M. Yogi, T. Nagai, Y. Imamura, H. Mukuda, Y. Kitaoka, D. Kikuchi, H. Sugawara, Y. Aoki, H. Sato, and H. Harima: J. Phys. Soc. Jpn. **75** (2006) 124702.
- 20) Y. Senga and H. Kontani: J. Phys. Soc. Jpn. **77** (2008) 113710.
- 21) Y. Senga and H. Kontani: New J. Phys. **11** (2009) 035005.
- 22) M. Matsumoto, M. Koga, and H. Kusunose: J. Phys. Soc. Jpn. **78** (2009) 084718.
- 23) J. Li and Y. Wang: Europhys. Lett. **88** (2009) 17009.
- 24) P. Fulde, L. L. Hirst, and A. Luther: Z. Phys. **230** (1970) 155.
- 25) J. Chang, I. Eremin, P. Thalmeier, and P. Fulde: Phys. Rev. B **76** (2007) 220510.
- 26) A. A. Abrikosov: Physics **2** (1965) 5.
- 27) H. Shul, B. T. Matthias, and L. R. Walker: Phys. Rev. Lett. **3** (1959) 552.
- 28) J. Kondo: Prog. Theor. Phys. **29** (1963) 1.
- 29) M. Koga and M. Matsumoto: Phys. Rev. B **77** (2008) 094411.
- 30) M. Koga and H. Shiba: J. Phys. Soc. Jpn. **64** (1995) 4345.
- 31) M. Koga, M. Matsumoto, and H. Shiba: J. Phys. Soc. Jpn. **75** (2006) 014709.
- 32) Y. Onodera and M. Okazaki: J. Phys. Soc. Jpn. **21** (1966) 2400.
- 33) K. Takegahara, H. Harima, and A. Yanase: J. Phys. Soc. Jpn. **70** (2001) 1190.
- 34) Y. Kuramoto, H. Kusunose, and A. Kiss: J. Phys. Soc. Jpn. **78** (2009) 072001.
- 35) Y. Aoki, T. Tayama, T. Sakakibara, K. Kuwahara, K. Izawa, M. Kohgi, W. Higemoto, D. E. MacLaughlin, H. Sugawara, and H. Sato: J. Phys. Soc. Jpn. **76** (2007) 051006.
- 36) M. Koga and H. Shiba: J. Phys. Soc. Jpn. **65** (1996) 3007.
- 37) S. Yotsuhashi, K. Miyake, and H. Kusunose: J. Phys. Soc. Jpn. **71** (2002) 389.
- 38) M. Koga and M. Matsumoto: J. Phys. Soc. Jpn. **76** (2007) 074714.
- 39) K. Yamaji and S. Abe: J. Phys. Soc. Jpn. **56** (1987) 4237.
- 40) Y. Yanagi, Y. Yamakawa, and Y. Ōno: Phys. Rev. B **81** (2010) 054518.